

## INVENTOR SEARCH

=> fil capl; d que nos l19

FILE 'CAPLUS' ENTERED AT 15:35:21 ON 12 MAR 2008

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FILE COVERS 1907 - 12 Mar 2008 VOL 148 ISS 11

FILE LAST UPDATED: 11 Mar 2008 (20080311/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

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L5          STR
L8          237 SEA FILE=REGISTRY SSS FUL L5
L9          4440 SEA FILE=CAPLUS ABB=ON  L8
L10         2 SEA FILE=CAPLUS ABB=ON  US2006-580588/AP
L11         273 SEA FILE=CAPLUS ABB=ON  SASHIDA Y?/AU
L12         285 SEA FILE=CAPLUS ABB=ON  MIMAKI Y?/AU
L13         2087 SEA FILE=CAPLUS ABB=ON  KURODA M?/AU
L14         1638 SEA FILE=CAPLUS ABB=ON  KOBAYASHI R?/AU
L15         36 SEA FILE=CAPLUS ABB=ON  KANDO H?/AU
L16         198 SEA FILE=CAPLUS ABB=ON  NOSAKA K?/AU
L17         4933 SEA FILE=CAPLUS ABB=ON  ISHII H?/AU
L18         243 SEA FILE=CAPLUS ABB=ON  YAMORI T?/AU
L19         3 SEA FILE=CAPLUS ABB=ON  (L10 OR L11 OR L12 OR L13 OR L14 OR
          L15 OR L16 OR L17 OR L18) AND L9

```

=> d ibib abs hitstr l19 1-3

L19 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:493610 CAPLUS Full-text

DOCUMENT NUMBER: 143:38374

TITLE: Antitumor activities of compounds from Compositae extracts

INVENTOR(S): Sashida, Yutaka; Mimaki, Yoshihiro  
; Kuroda, Minpei; Kobayashi, Ryosuke  
; Kando, Hiroaki; Nosaka, Kosuke;  
Ishii, Hiroyasu; Yamori, Takao

PATENT ASSIGNEE(S): Hiro International Co., Ltd., Japan

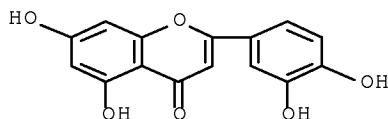
SOURCE: PCT Int. Appl., 44 pp.

CODEN: PIXXD2

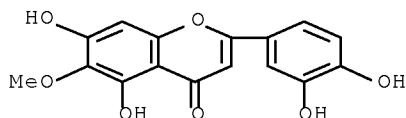
DOCUMENT TYPE: Patent

LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051955	A1	20050609	WO 2004-JP17480	20041125
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005179339	A	20050707	JP 2004-265620	20040913
JP 3816504	B2	20060830		
EP 1688419	A1	20060809	EP 2004-819399	20041125
R: DE, FR, GB				
JP 2005232192	A	20050902	JP 2005-144115	20050517
JP 2005272477	A	20051006	JP 2005-144077	20050517
JP 2005298516	A	20051027	JP 2005-144092	20050517
US 2007129427	A1	20070607	US 2006-580588	20060525 <--
PRIORITY APPLN. INFO.:			JP 2003-397647	A 20031127
			JP 2004-265620	A 20040913
			WO 2004-JP17480	W 20041125
AB	Disclosed are novel compds. extracted and isolated from a plant belonging to Compositae. Compds., such as (1S,3R,4S,6R,7S,8R,10R)-1-hydroxy-3-methoxy-3,10-epoxy-8-isobutyryloxygermacra-11(13)-en-6,12-olide, (4S,5R)-4-hydroxy-4-[(1E,3S)-3-hydroxy-1-butenyl]-3,3,5-trimethylcyclohexanone, and (1S,3R,6R,7R,8R,10R)-1-hydroxy-3-methoxy-3,10-epoxy-8-isobutyryloxygermacra-4,11(13)-en-6,12-olide, were identified from the exts. and in vitro antitumor activities against human acute lymphoid leukemia cell (HL-60) were tested.			
IT	491-70-3P, Luteolin 520-11-6P, Nepetin 56377-67-4P 59979-56-5P 59979-57-6P, Tagitinin F 59979-58-7P 59979-61-2P 110382-31-5P 110382-36-0P 194474-71-0P 853273-93-5P 853273-94-6P 853273-95-7P			
	RL: PAC (Pharmacological activity); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation) (antitumor activities of compds. from Compositae exts.)			
RN	491-70-3 CAPLUS			
CN	4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)			

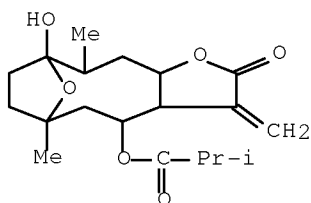


RN 520-11-6 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-methoxy- (CA INDEX NAME)



RN 56377-67-4 CAPLUS

CN Propanoic acid, 2-methyl-, (3aS,4R,6S,9R,10S,11aR)-dodecahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (9CI) (CA INDEX NAME)

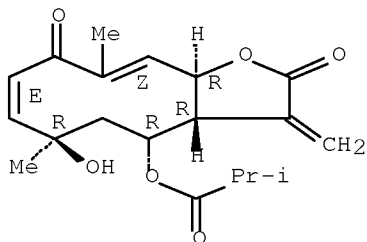


RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.

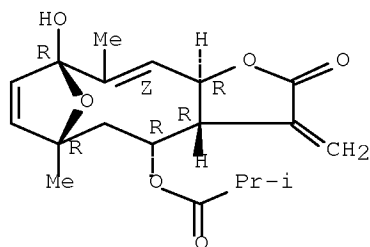


RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

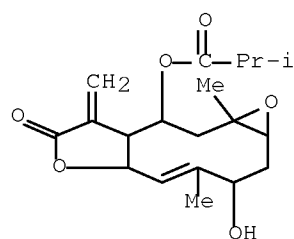
Absolute stereochemistry.

Double bond geometry as described by E or Z.



RN 59979-58-7 CAPLUS

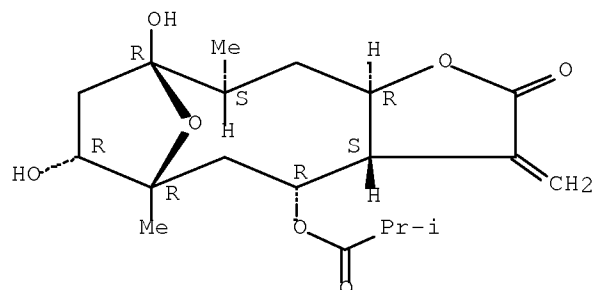
CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



RN 59979-61-2 CAPLUS

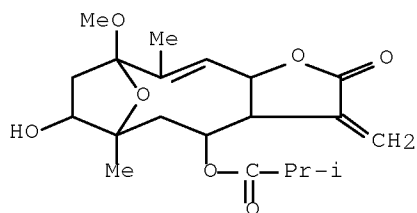
CN Propanoic acid, 2-methyl-, (3aS,4R,6R,7R,9R,10S,11aR)-dodecahydro-7,9-dihydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.



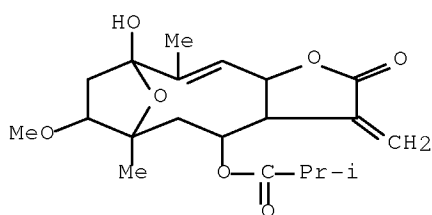
RN 110382-31-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7R,9R,10Z,11aR)-2,3,3a,4,5,6,7,8,9,11a-decahydro-7-hydroxy-9-methoxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (9CI) (CA INDEX NAME)



RN 110382-36-0 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7R,9R,10Z,11aR)-2,3,3a,4,5,6,7,8,9,11a-decahydro-9-hydroxy-7-methoxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (9CI) (CA INDEX NAME)



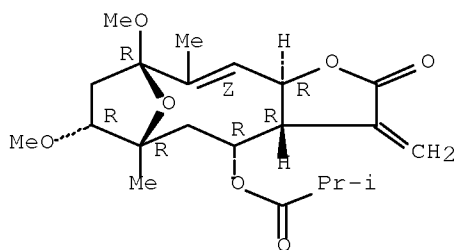
RN 194474-71-0 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7R,9R,10Z,11aR)-2,3,3a,4,5,6,7,8,9,11a-decahydro-7,9-dimethoxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as described by E or Z.

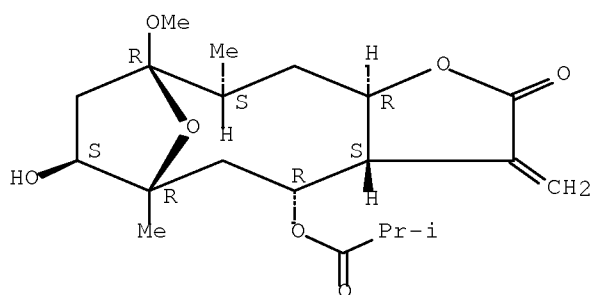
Currently available stereo shown.



RN 853273-93-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aS,4R,6R,7S,9R,10S,11aR)-dodecahydro-7-hydroxy-9-methoxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

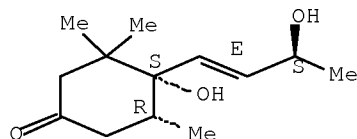
Absolute stereochemistry. Rotation (-).



RN 853273-94-6 CAPLUS

CN Cyclohexanone, 4-hydroxy-4-[(1E,3S)-3-hydroxy-1-butenyl]-3,3,5-trimethyl-, (4S,5R)- (9CI) (CA INDEX NAME)

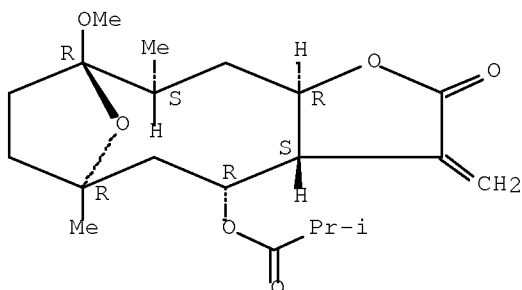
Absolute stereochemistry. Rotation (-).  
Double bond geometry as shown.



RN 853273-95-7 CAPLUS

CN Propanoic acid, 2-methyl-, (3aS,4R,6R,9R,10S,11aR)-dodecahydro-9-methoxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

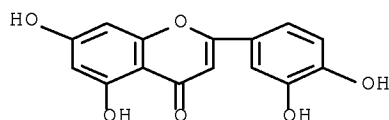
ACCESSION NUMBER: 1992:466580 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 117:66580

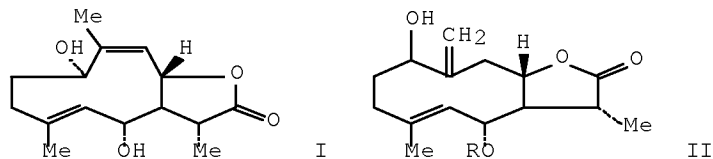
TITLE: New acylated glucosides of chalcone from the leaves of *Bidens frondosa*

AUTHOR(S): Karikome, Hiroyuki; Ogawa, Kazunori; Sashida, Yutaka

CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1992), 40(3), 689-91  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 117:66580  
 AB Five new acylated glucosides of okanin [okanin 4-O-(6''-O-acetyl-2''-O-caffeoyl- $\beta$ -D-glucopyranoside), okanin 4-O-(2''-caffeoyl-6''-p- coumaroyl- $\beta$ -D-glucopyranoside), 4-O-methylokanin 4'-O-(6''-O-p- coumaroyl- $\beta$ -D-glucopyranoside), 4-O-methylokanin 4'-O-acetyl- $\beta$ -D- glucopyranoside), and 4-O-methylokanin 4'-O-(6'-O-acetyl-2''-O-caffeoyl-  $\beta$ -D-glucopyranoside)], have been isolated from the fresh leaves of *Bidens frondosa*. These structures have been elucidated on the basis of spectral data and chemical correlation.  
 IT 491-70-3, Luteolin  
 RL: BIOL (Biological study)  
 (from *Bidens frondosa*)  
 RN 491-70-3 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



L19 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1984:20391 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 100:20391  
 ORIGINAL REFERENCE NO.: 100:3171a,3174a  
 TITLE: Sesquiterpene lactones from pyrethrum flowers  
 AUTHOR(S): Sashida, Yutaka; Nakata, Hiroyuki;  
 Shimomura, Hiroko; Kagaya, Mitsuko  
 CORPORATE SOURCE: Tokyo Coll. Pharm., Tokyo, 192, Japan  
 SOURCE: Phytochemistry (Elsevier) (1983), 22(5), 1219-22  
 CODEN: PYTCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The new sesquiterpene lactones I and II (R = H or 1- $\beta$ -D-glycosyl), together with the known sesquiterpene lactones tatridin-A, -B, and dihydro- $\beta$ -

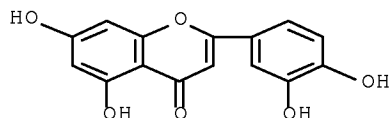
cyclopyrethrosin, and the known flavonoids jaceidin, apigenin, luteolin, apigenin-7-galacturonic acid Me ester, and apigenin-7-glucuronic acid were isolated from the flowers of *Chrysanthemum cinerariaefolium*. The structures of I and II were determined by standard chemical and spectral methods. All the compds. isolated inhibited the root growth of Chinese cabbage seedlings.

IT 491-70-3

RL: BIOL (Biological study)  
(from *Chrysanthemum cinerariaefolium*)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



## STRUCTURE SEARCH

=> fil reg; d stat que 144; d stat que 149; d que nos 153; d que nos 163  
FILE 'REGISTRY' ENTERED AT 15:36:28 ON 12 MAR 2008  
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STRUCTURE FILE UPDATES: 11 MAR 2008 HIGHEST RN 1007457-12-6  
DICTIONARY FILE UPDATES: 11 MAR 2008 HIGHEST RN 1007457-12-6

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REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

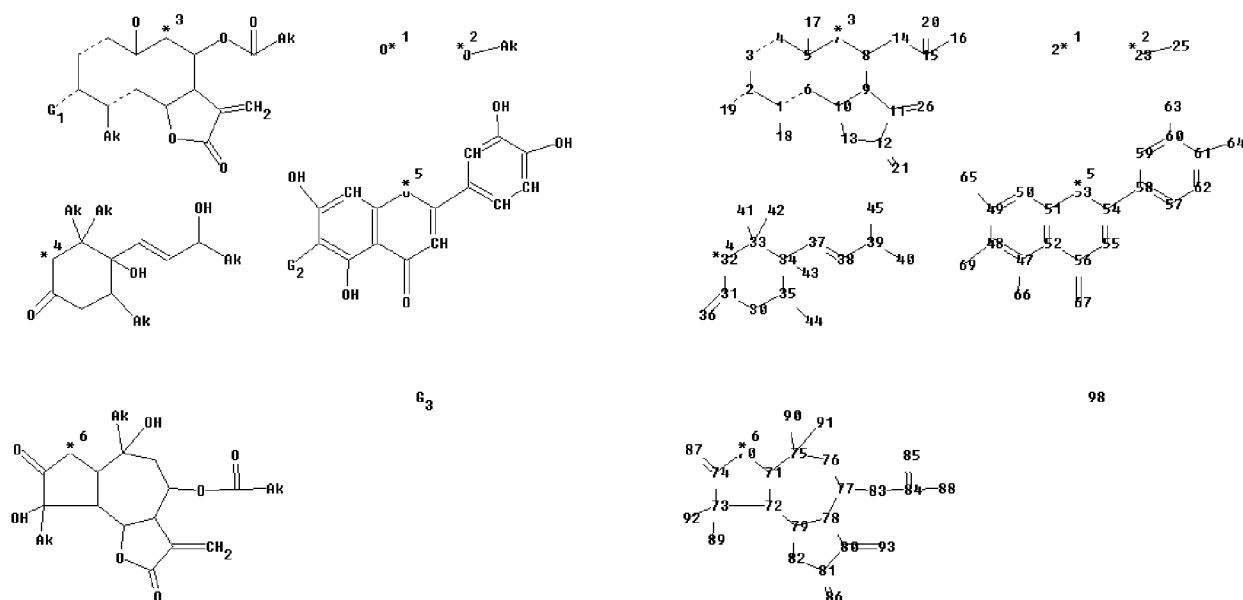
<http://www.cas.org/support/stngen/stdoc/properties.html>

L5 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

Uploading L5.str



chain nodes :

14 15 16 18 19 20 21 22 23 25 26 36 37 38 39 40 41 42 43 44 45  
63 64 65 66 67 69 83 84 85 86 87 88 89 90 91 92 93 98

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 30 31 32 33 34 35 47 48 49 50  
51 52 53 54 55 56 57 58 59 60 61 62 70 71 72 73 74 75 76 77 78  
79 80 81 82

ring/chain nodes :

17

chain bonds :

1-18 2-19 8-14 11-26 12-21 14-15 15-16 15-20 23-25 31-36 33-41 33-42  
34-37 34-43 35-44 37-38 38-39 39-40 39-45 47-66 48-69 49-65 54-58 56-67  
60-63 61-64 73-89 73-92 74-87 75-90 75-91 77-83 80-93 81-86 83-84 84-85  
84-88

ring/chain bonds :

5-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-7 6-10 7-8 8-9 9-10 9-11 10-13 11-12 12-13 30-  
31 30-35 31-32 32-33 33-34 34-35 47-48 47-52 48-49 49-50 50-51 51-52  
51-53 52-56 53-54 54-55 55-56 57-58 57-62 58-59 59-60 60-61 61-62 70-71  
70-74 71-72 71-75 72-73 72-79 73-74 75-76 76-77 77-78 78-79 78-80 79-82  
80-81 81-82

exact/norm bonds :

1-2 1-6 1-18 2-3 2-19 3-4 4-5 5-7 6-10 7-8 8-9 8-14 9-10 9-11 10-13  
11-12 12-13 12-21 14-15 15-16 15-20 23-25 31-36 33-41 33-42 34-43 35-44  
39-40 39-45 47-66 48-69 49-65 51-53 52-56 53-54 54-55 55-56 56-67 60-63  
61-64 70-71 70-74 71-72 71-75 72-73 72-79 73-74 73-89 73-92 74-87 75-76  
75-90 75-91 76-77 77-78 77-83 78-79 78-80 79-82 80-81 81-82 81-86 83-84  
84-85 84-88

exact bonds :

5-17 11-26 30-31 30-35 31-32 32-33 33-34 34-35 34-37 37-38 38-39 54-58  
80-93

normalized bonds :

47-48 47-52 48-49 49-50 50-51 51-52 57-58 57-62 58-59 59-60 60-61 61-62

G1:[\*1],[\*2]

G2:H,MeO

G3:[\*3],[\*4],[\*5],[\*6]

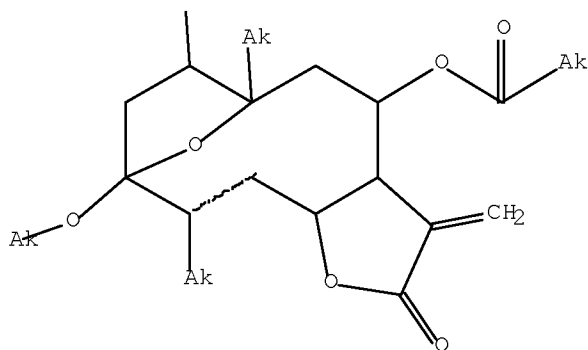
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25:1 E exact RC ring/chain 40:1 E exact RC ring/chain 41:1 E exact RC ring/chain  
42:1 E exact RC ring/chain 44:1 E exact RC ring/chain 88:1 E exact RC ring/chain  
89:1 E exact RC ring/chain 90:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:CLASS 30:Atom  
31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:CLASS 37:CLASS 38:CLASS 39:CLASS  
40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 47:Atom 48:Atom  
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom  
58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 64:CLASS 65:CLASS 66:CLASS  
67:CLASS 69:CLASS 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom  
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:CLASS 84:CLASS 85:CLASS  
86:CLASS 87:CLASS 88:CLASS 89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS  
98:CLASS

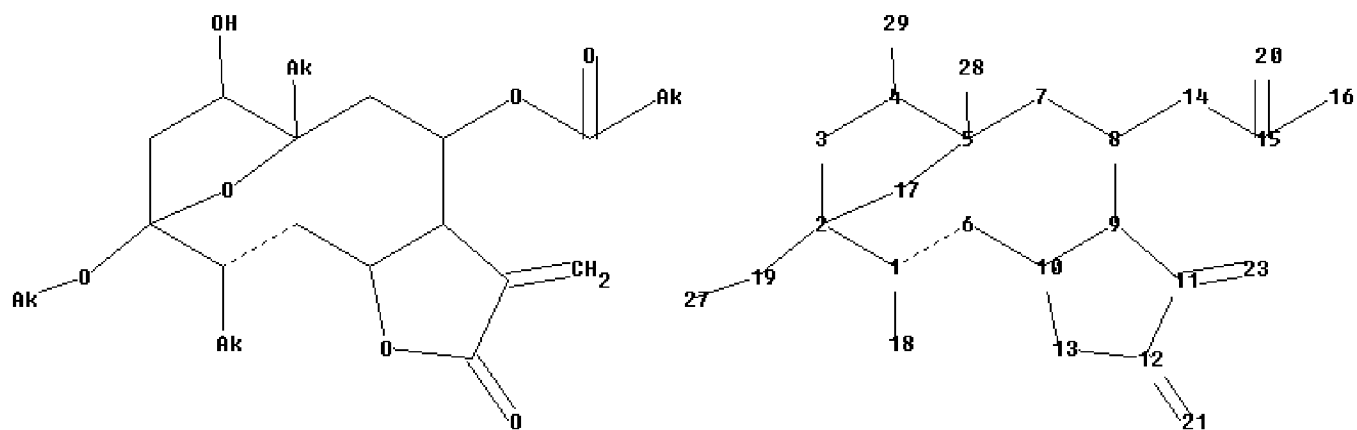
L8 237 SEA FILE=REGISTRY SSS FUL L5  
L35 STR



G1  
G2 H,MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L35.str



```

chain nodes :
14 15 16 18 19 20 21 23 27 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 17
chain bonds :
1-18 2-19 4-29 5-28 8-14 11-23 12-21 14-15 15-16 15-20 19-27
ring bonds :
1-2 1-6 2-3 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12
12-13
exact/norm bonds :
1-6 1-18 3-4 5-28 8-14 14-15 15-16 15-20 19-27
exact bonds :
1-2 2-3 2-19 2-17 4-5 4-29 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-
12 11-23 12-13 12-21
isolated ring systems :
containing 1 :

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G1

G2:H,MeO

G3

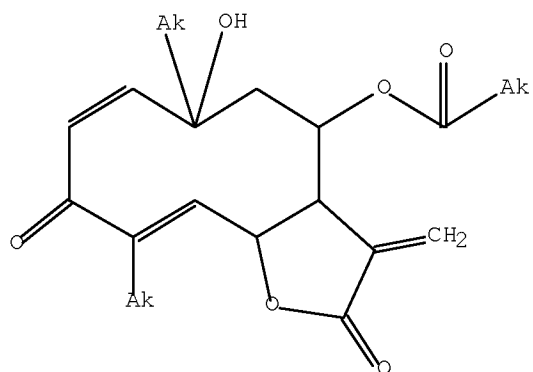
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Connectivity :
1:3 E exact RC ring/chain 6:2 E exact RC ring/chain 16:1 E exact RC ring/chain
18:1 E exact RC ring/chain 27:1 E exact RC ring/chain 28:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS 28:CLASS 29:CLASS

```

L36

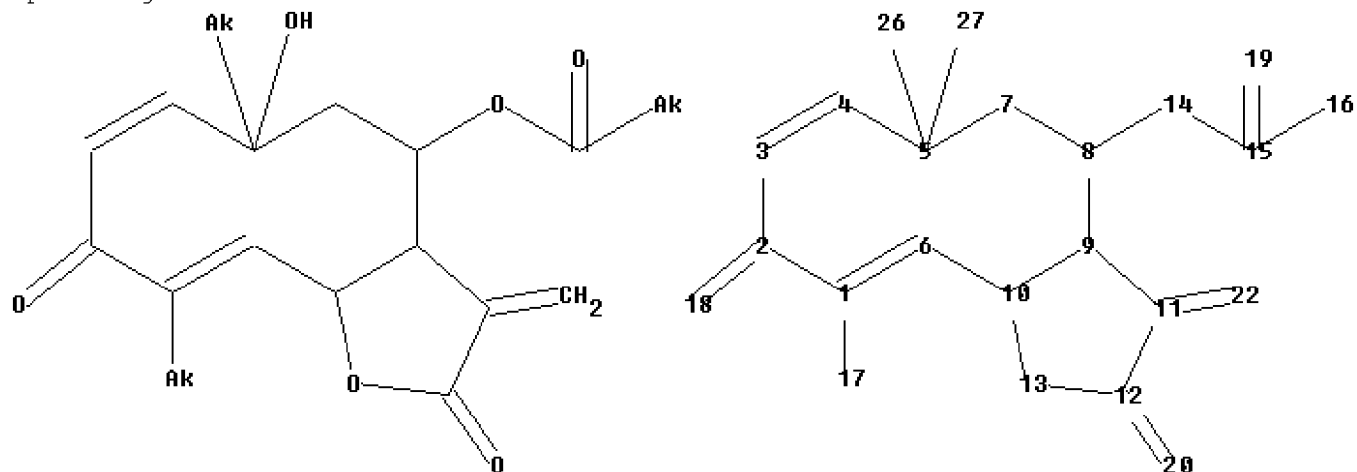
STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L36.str



chain nodes :  
14 15 16 17 18 19 20 22 26 27  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12 13  
chain bonds :  
1-17 2-18 5-26 5-27 8-14 11-22 12-20 14-15 15-16 15-19  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-7 6-10 7-8 8-9 9-10 9-11 10-13 11-12 12-13  
exact/norm bonds :  
1-17 2-18 5-26 8-14 12-20 14-15 15-16 15-19  
exact bonds :  
1-2 1-6 2-3 3-4 4-5 5-7 5-27 6-10 7-8 8-9 9-10 9-11 10-13 11-12 11-22  
12-13  
isolated ring systems :  
containing 1 :

G1

G2:H, MeO

G3

Connectivity :

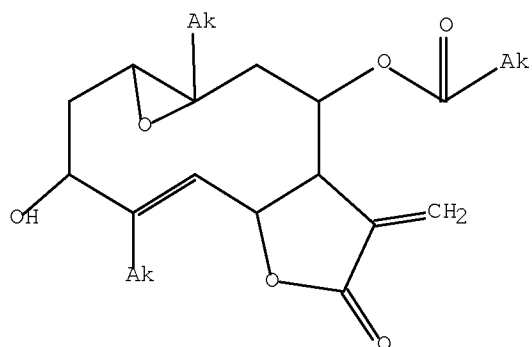
16:1 E exact RC ring/chain 17:1 E exact RC ring/chain 18:1 E exact RC ring/chain  
 26:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 22:CLASS 26:CLASS 27:CLASS

L37

STR



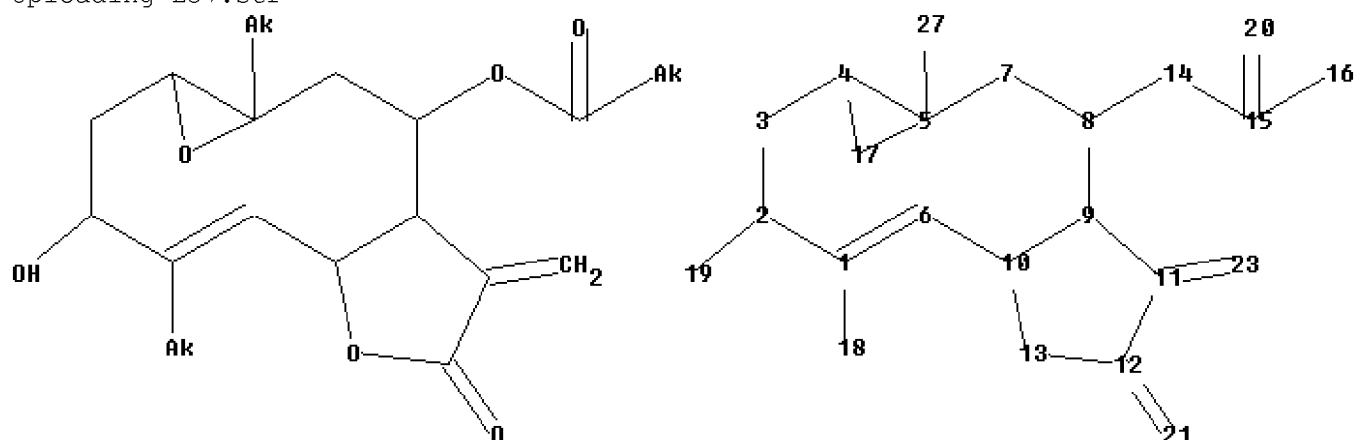
G1

G2 H, MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L37.str



chain nodes :

14 15 16 18 19 20 21 23 27

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 17

chain bonds :

1-18 2-19 5-27 8-14 11-23 12-21 14-15 15-16 15-20

ring bonds :  
 1-2 1-6 2-3 3-4 4-5 4-17 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12  
 12-13  
 exact/norm bonds :  
 1-18 5-27 8-14 14-15 15-16 15-20  
 exact bonds :  
 1-2 1-6 2-3 2-19 3-4 4-5 4-17 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13  
 11-12 11-23 12-13 12-21  
 isolated ring systems :  
 containing 1 :

G1

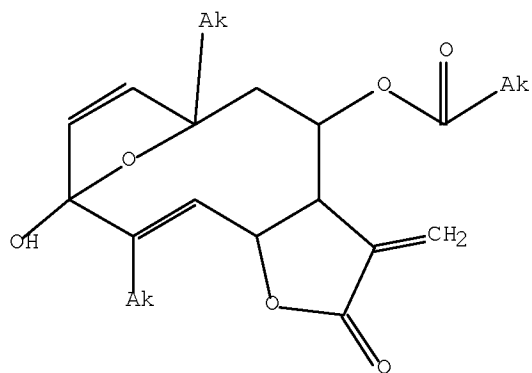
G2:H,MeO

G3

Connectivity :  
 16:1 E exact RC ring/chain 18:1 E exact RC ring/chain 27:1 E exact RC ring/chain  
 Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS

L38

STR



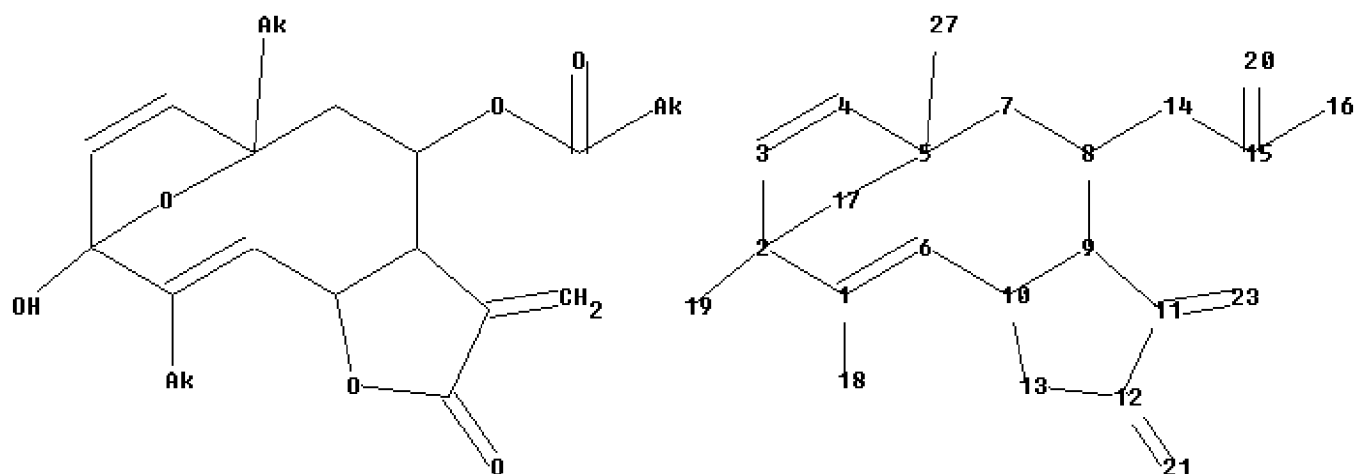
G1

G2 H,MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L38.str



```

chain nodes :
14 15 16 18 19 20 21 23 27
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 17
chain bonds :
1-18 2-19 5-27 8-14 11-23 12-21 14-15 15-16 15-20
ring bonds :
1-2 1-6 2-3 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12
12-13
exact/norm bonds :
1-18 5-27 8-14 14-15 15-16 15-20
exact bonds :
1-2 1-6 2-3 2-19 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13
11-12 11-23 12-13 12-21
isolated ring systems :
containing 1 :

```

G1

G2:H, MeO

G3

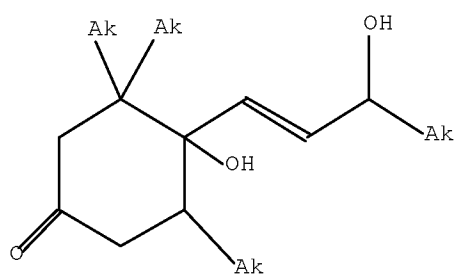
```

Connectivity :
16:1 E exact RC ring/chain 18:1 E exact RC ring/chain 27:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS

```

L39

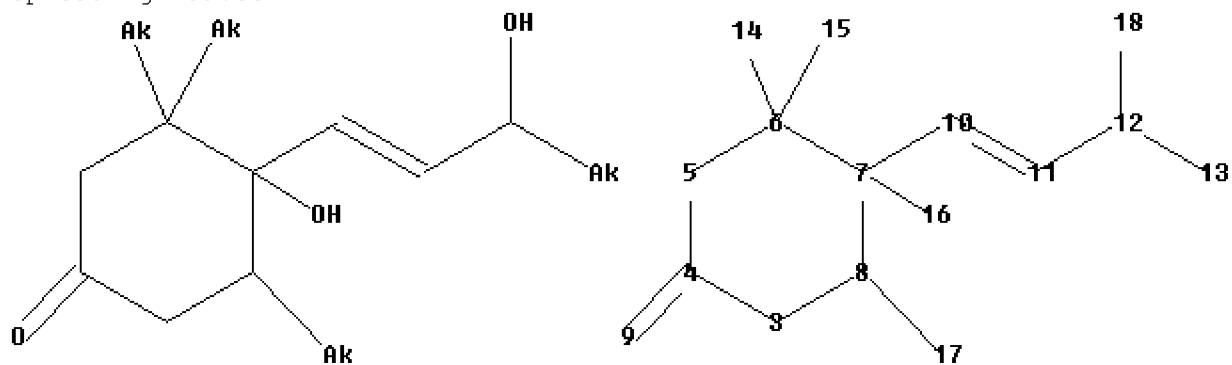
STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L39.str



```
chain nodes :
9 10 11 12 13 14 15 16 17 18
ring nodes :
3 4 5 6 7 8
chain bonds :
4-9 6-14 6-15 7-10 7-16 8-17 10-11 11-12 12-13 12-18
ring bonds :
3-4 3-8 4-5 5-6 6-7 7-8
exact/norm bonds :
4-9 6-14 6-15 8-17 12-13
exact bonds :
3-4 3-8 4-5 5-6 6-7 7-8 7-10 7-16 10-11 11-12 12-18
isolated ring systems :
containing 3 :
```

G1

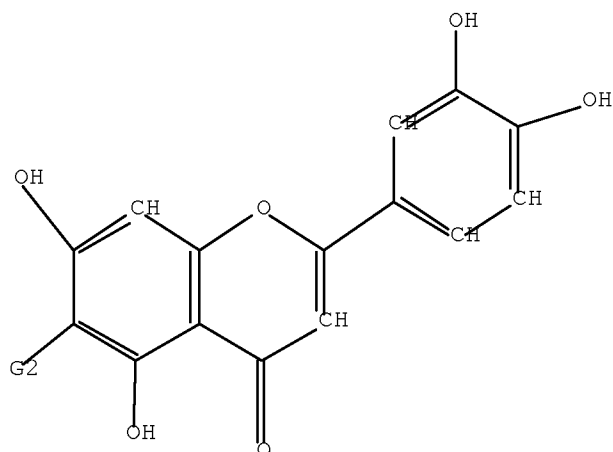
G2:H, MeO

G3

```
Connectivity :
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:1 E exact RC ring/chain
17:1 E exact RC ring/chain
Match level :
3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:CLASS
```

12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

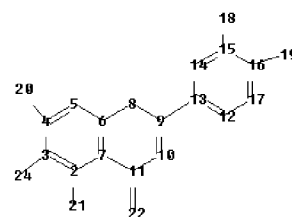
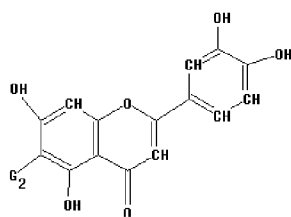
L40 STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L40.str



chain nodes :  
18 19 20 21 22 24  
ring nodes :  
2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17  
chain bonds :  
2-21 3-24 4-20 9-13 11-22 15-18 16-19  
ring bonds :  
2-3 2-7 3-4 4-5 5-6 6-7 6-8 7-11 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17  
exact/norm bonds :

2-21 3-24 4-20 11-22 15-18 16-19

exact bonds :

6-8 7-11 8-9 9-10 9-13 10-11

normalized bonds :

2-3 2-7 3-4 4-5 5-6 6-7 12-13 12-17 13-14 14-15 15-16 16-17

isolated ring systems :

containing 2 : 12 :

G1

G2:H, MeO

G3

Match level :

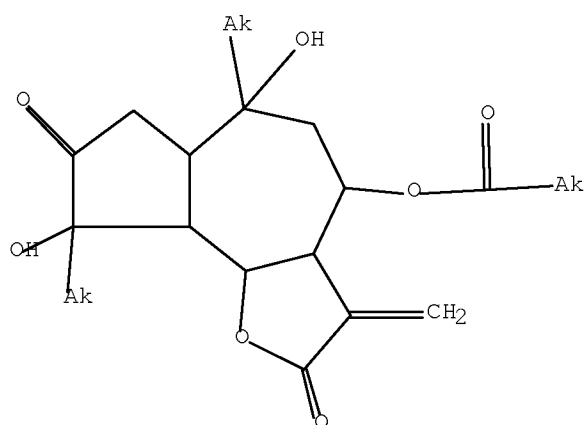
2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS

21:CLASS 22:CLASS 24:CLASS

L41

STR



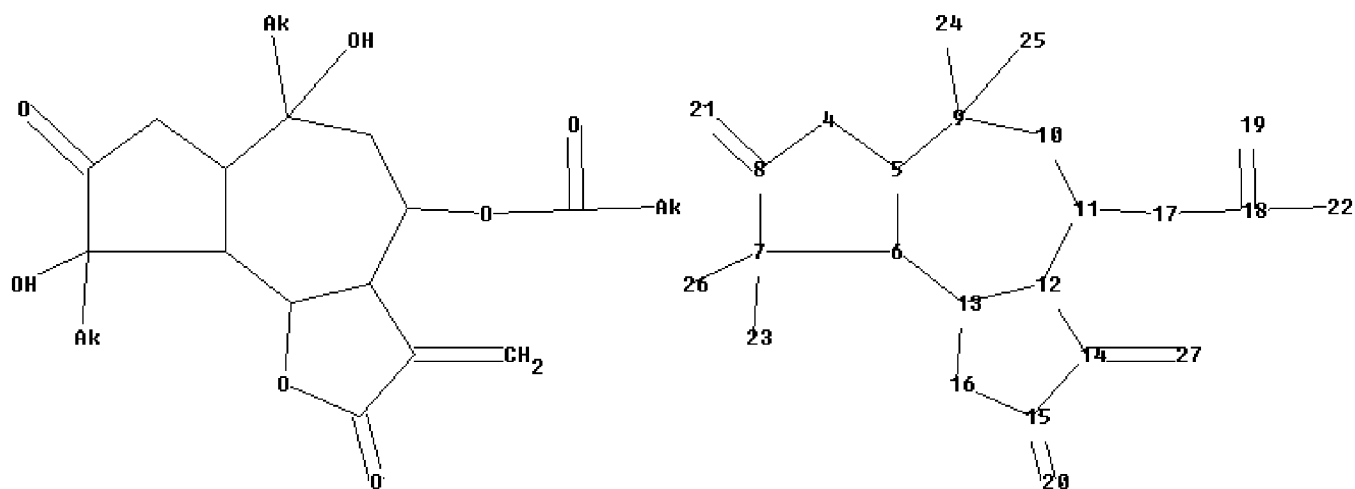
G1

G2 H, MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L41.str



```

chain nodes :
17 18 19 20 21 22 23 24 25 26 27
ring nodes :
4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
7-23 7-26 8-21 9-24 9-25 11-17 14-27 15-20 17-18 18-19 18-22
ring bonds :
4-5 4-8 5-6 5-9 6-7 6-13 7-8 9-10 10-11 11-12 12-13 12-14 13-16 14-15
15-16
exact/norm bonds :
7-23 8-21 9-24 11-17 15-20 17-18 18-19 18-22
exact bonds :
4-5 4-8 5-6 5-9 6-7 6-13 7-8 7-26 9-10 9-25 10-11 11-12 12-13 12-14
13-16 14-15 14-27 15-16
isolated ring systems :
containing 4 :
```

G1

G2:H, MeO

G3

```

Connectivity :
22:1 E exact RC ring/chain 23:1E exact RC ring/chain 24:1 E exact RC ring/chain
Match level :
4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
```

```

L44          65 SEA FILE=REGISTRY SUB=L8 SSS FUL (L35 OR L36 OR L37 OR L38 OR
              L39 OR L40 OR L41)
```

```

100.0% PROCESSED      181 ITERATIONS
SEARCH TIME: 00.00.01
```

65 ANSWERS

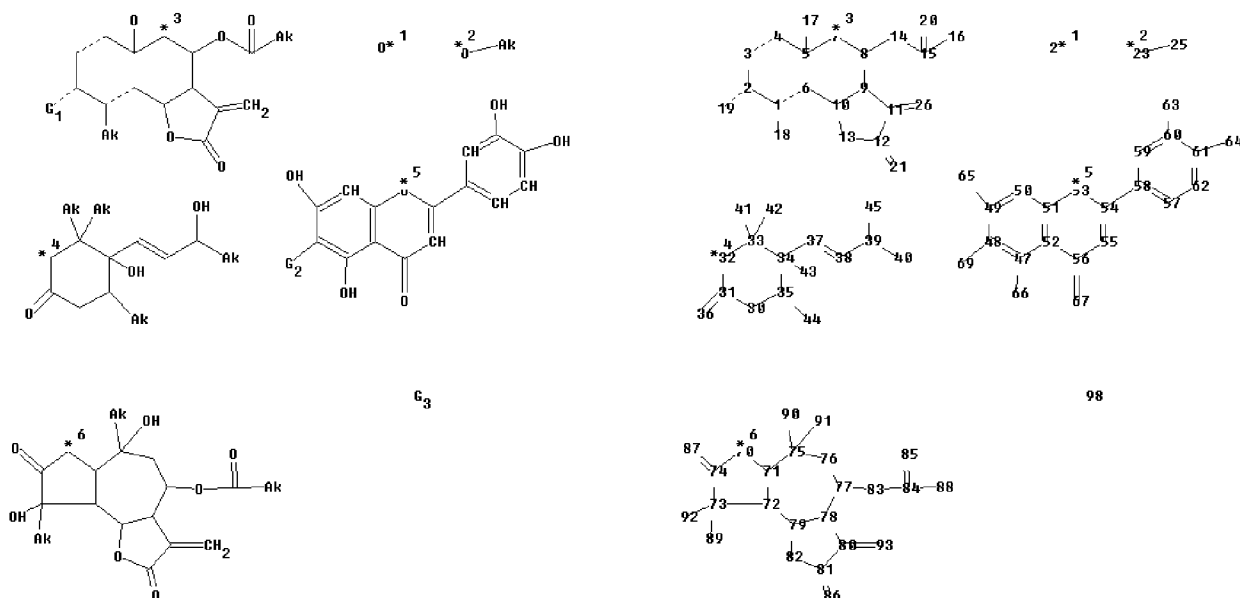
L5

STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

Uploading L5.str



chain nodes :

14 15 16 18 19 20 21 22 23 25 26 36 37 38 39 40 41 42 43 44 45  
63 64 65 66 67 69 83 84 85 86 87 88 89 90 91 92 93 98

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 30 31 32 33 34 35 47 48 49 50  
51 52 53 54 55 56 57 58 59 60 61 62 70 71 72 73 74 75 76 77 78  
79 80 81 82

ring/chain nodes :

17

chain bonds :

1-18 2-19 8-14 11-26 12-21 14-15 15-16 15-20 23-25 31-36 33-41 33-42  
34-37 34-43 35-44 37-38 38-39 39-40 39-45 47-66 48-69 49-65 54-58 56-67  
60-63 61-64 73-89 73-92 74-87 75-90 75-91 77-83 80-93 81-86 83-84 84-85  
84-88

ring/chain bonds :

5-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-7 6-10 7-8 8-9 9-10 9-11 10-13 11-12 12-13 30-  
31 30-35 31-32 32-33 33-34 34-35 47-48 47-52 48-49 49-50 50-51 51-52  
51-53 52-56 53-54 54-55 55-56 57-58 57-62 58-59 59-60 60-61 61-62 70-71  
70-74 71-72 71-75 72-73 72-79 73-74 75-76 76-77 77-78 78-79 78-80 79-82  
80-81 81-82

exact/norm bonds :

1-2 1-6 1-18 2-3 2-19 3-4 4-5 5-7 6-10 7-8 8-9 8-14 9-10 9-11 10-13  
11-12 12-13 12-21 14-15 15-16 15-20 23-25 31-36 33-41 33-42 34-43 35-44  
39-40 39-45 47-66 48-69 49-65 51-53 52-56 53-54 54-55 55-56 56-67 60-63

61-64 70-71 70-74 71-72 71-75 72-73 72-79 73-74 73-89 73-92 74-87 75-76  
 75-90 75-91 76-77 77-78 77-83 78-79 78-80 79-82 80-81 81-82 81-86 83-84  
 84-85 84-88

exact bonds :

5-17 11-26 30-31 30-35 31-32 32-33 33-34 34-35 34-37 37-38 38-39 54-58  
 80-93

normalized bonds :

47-48 47-52 48-49 49-50 50-51 51-52 57-58 57-62 58-59 59-60 60-61 61-62

G1:[\*1],[\*2]

G2:H,MeO

G3:[\*3],[\*4],[\*5],[\*6]

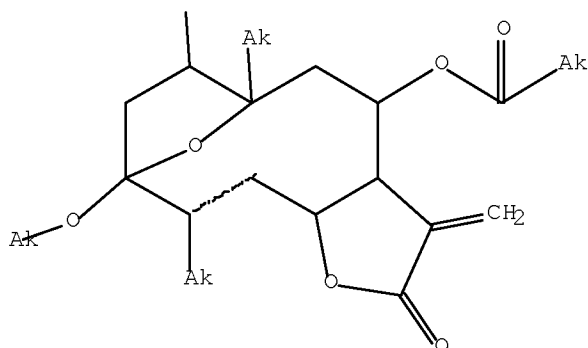
Connectivity :

16:1 E exact RC ring/chain 18:1 E exact RC ring/chain 22:1 E exact RC ring/chain  
 25:1 E exact RC ring/chain 40:1 E exact RC ring/chain 41:1 E exact RC ring/chain  
 42:1 E exact RC ring/chain 44:1 E exact RC ring/chain 88:1 E exact RC ring/chain  
 89:1 E exact RC ring/chain 90:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:CLASS 30:Atom  
 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:CLASS 37:CLASS 38:CLASS 39:CLASS  
 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 47:Atom 48:Atom  
 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom  
 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 64:CLASS 65:CLASS 66:CLASS  
 67:CLASS 69:CLASS 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom  
 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:CLASS 84:CLASS 85:CLASS  
 86:CLASS 87:CLASS 88:CLASS 89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS  
 98:CLASS

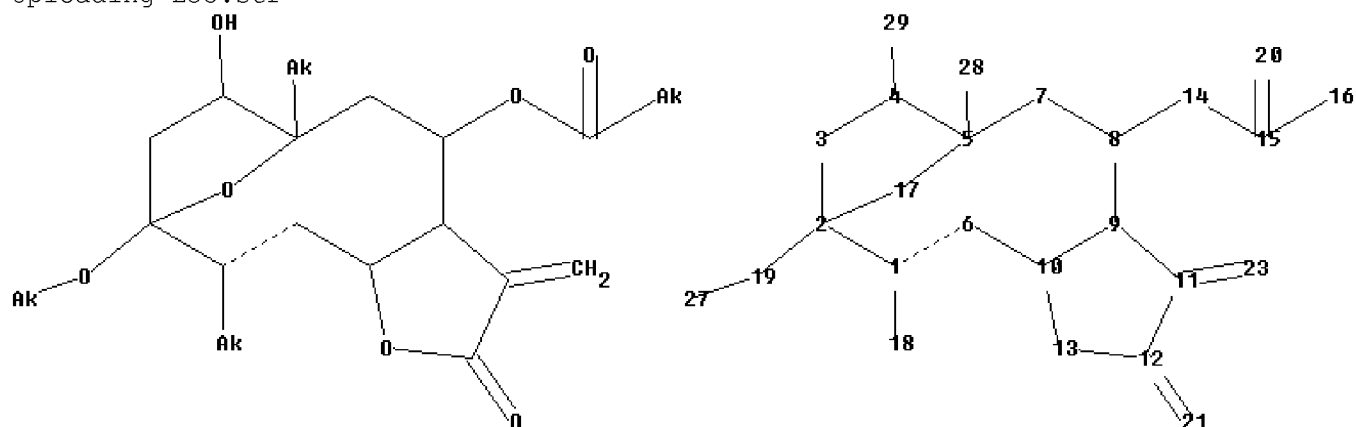
L8 237 SEA FILE=REGISTRY SSS FUL L5  
 L35 STR



G1  
 G2 H,MeO  
 G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L35.str



```

chain nodes :
14 15 16 18 19 20 21 23 27 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 17
chain bonds :
1-18 2-19 4-29 5-28 8-14 11-23 12-21 14-15 15-16 15-20 19-27
ring bonds :
1-2 1-6 2-3 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12
12-13
exact/norm bonds :
1-6 1-18 3-4 5-28 8-14 14-15 15-16 15-20 19-27
exact bonds :
1-2 2-3 2-19 2-17 4-5 4-29 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-
12 11-23 12-13 12-21
isolated ring systems :
containing 1 :

```

G1

G2:H, MeO

G3

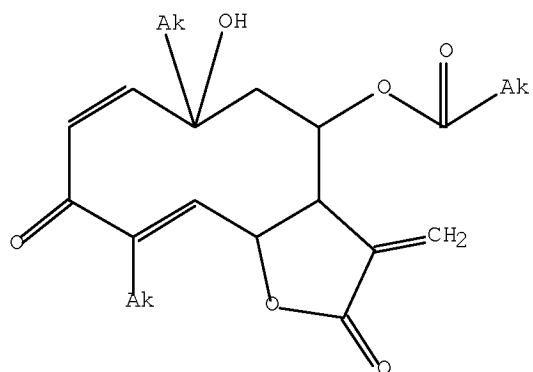
```

Connectivity :
1:3 E exact RC ring/chain 6:2 E exact RC ring/chain 16:1 E exact RC ring/chain
18:1 E exact RC ring/chain 27:1 E exact RC ring/chain 28:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS 28:CLASS 29:CLASS

```

L36

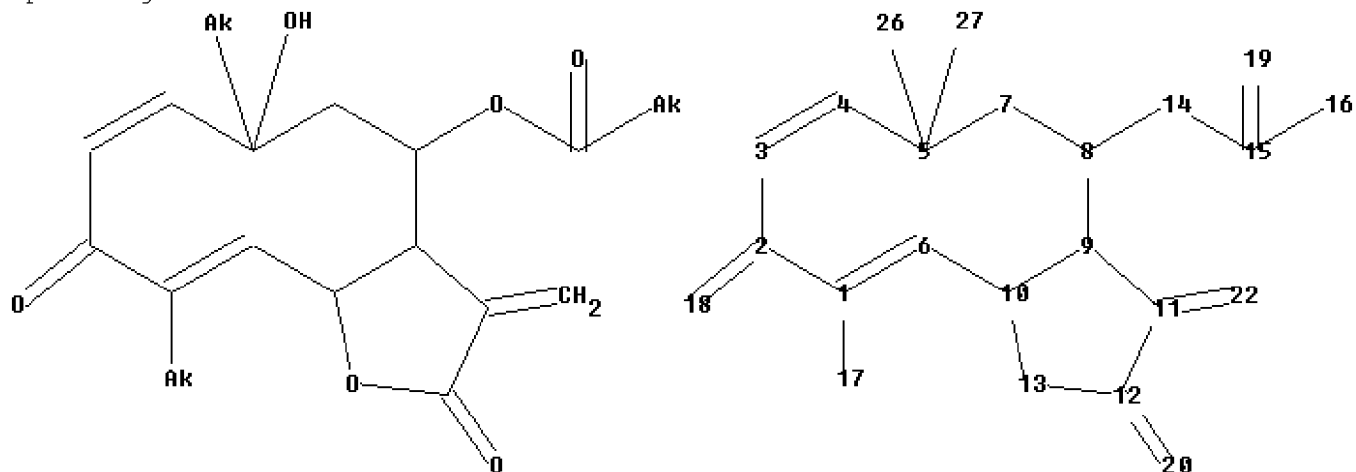
STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L36.str



chain nodes :  
14 15 16 17 18 19 20 22 26 27  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12 13  
chain bonds :  
1-17 2-18 5-26 5-27 8-14 11-22 12-20 14-15 15-16 15-19  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-7 6-10 7-8 8-9 9-10 9-11 10-13 11-12 12-13  
exact/norm bonds :  
1-17 2-18 5-26 8-14 12-20 14-15 15-16 15-19  
exact bonds :  
1-2 1-6 2-3 3-4 4-5 5-7 5-27 6-10 7-8 8-9 9-10 9-11 10-13 11-12 11-22  
12-13  
isolated ring systems :  
containing 1 :

G1

G2:H, MeO

G3

Connectivity :

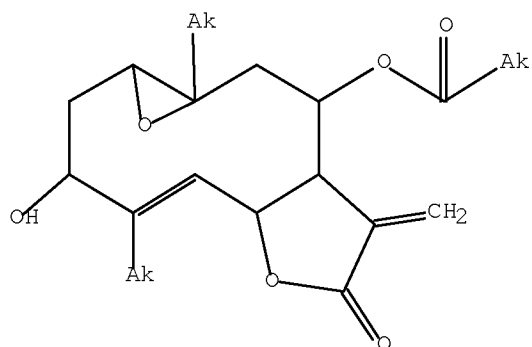
16:1 E exact RC ring/chain 17:1 E exact RC ring/chain 18:1 E exact RC ring/chain  
 26:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 22:CLASS 26:CLASS 27:CLASS

L37

STR



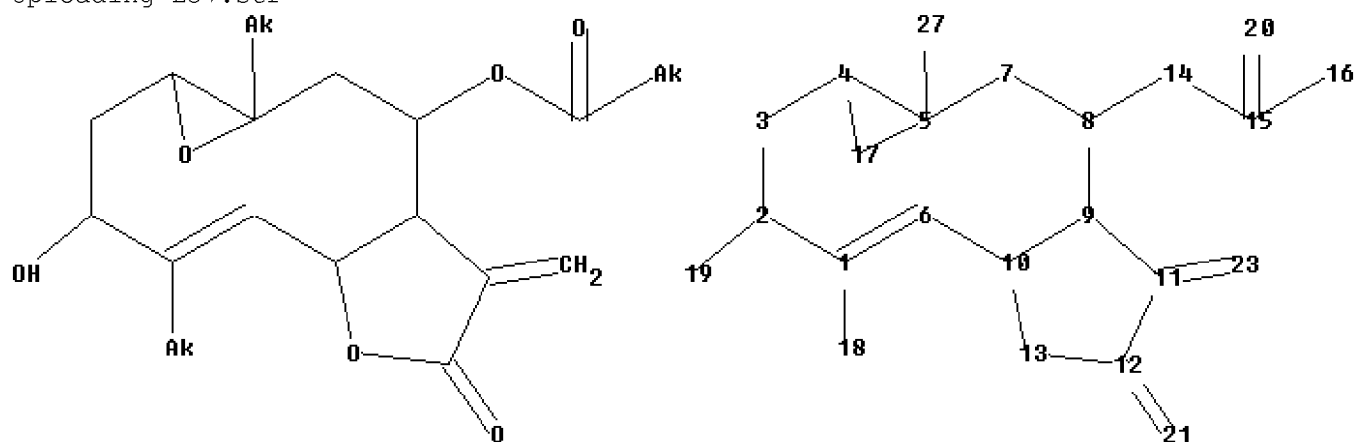
G1

G2 H, MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L37.str



chain nodes :

14 15 16 18 19 20 21 23 27

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 17

chain bonds :

1-18 2-19 5-27 8-14 11-23 12-21 14-15 15-16 15-20

ring bonds :  
 1-2 1-6 2-3 3-4 4-5 4-17 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12  
 12-13  
 exact/norm bonds :  
 1-18 5-27 8-14 14-15 15-16 15-20  
 exact bonds :  
 1-2 1-6 2-3 2-19 3-4 4-5 4-17 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13  
 11-12 11-23 12-13 12-21  
 isolated ring systems :  
 containing 1 :

G1

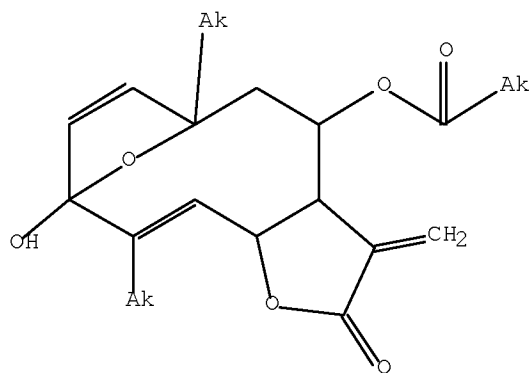
G2:H,MeO

G3

Connectivity :  
 16:1 E exact RC ring/chain 18:1 E exact RC ring/chain 27:1 E exact RC ring/chain  
 Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS

L38

STR



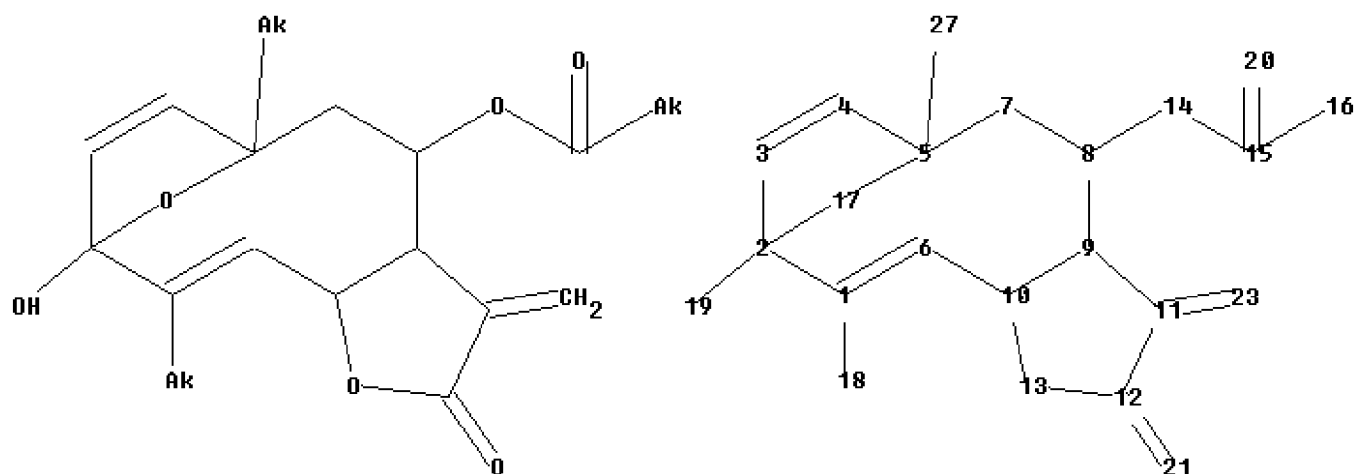
G1

G2 H,MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L38.str



```

chain nodes :
14 15 16 18 19 20 21 23 27
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 17
chain bonds :
1-18 2-19 5-27 8-14 11-23 12-21 14-15 15-16 15-20
ring bonds :
1-2 1-6 2-3 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12
12-13
exact/norm bonds :
1-18 5-27 8-14 14-15 15-16 15-20
exact bonds :
1-2 1-6 2-3 2-19 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13
11-12 11-23 12-13 12-21
isolated ring systems :
containing 1 :

```

G1

G2:H, MeO

G3

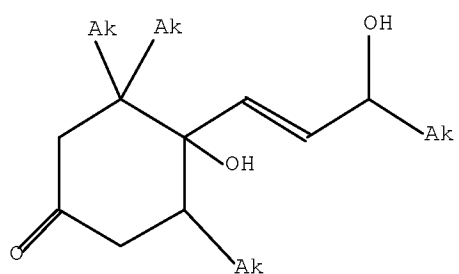
```

Connectivity :
16:1 E exact RC ring/chain 18:1 E exact RC ring/chain 27:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS

```

L39

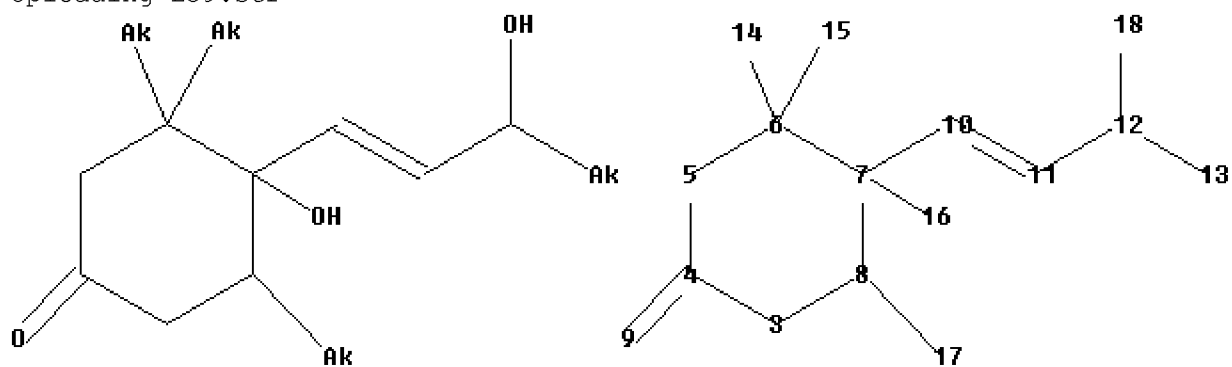
STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L39.str



chain nodes :  
9 10 11 12 13 14 15 16 17 18  
ring nodes :  
3 4 5 6 7 8  
chain bonds :  
4-9 6-14 6-15 7-10 7-16 8-17 10-11 11-12 12-13 12-18  
ring bonds :  
3-4 3-8 4-5 5-6 6-7 7-8  
exact/norm bonds :  
4-9 6-14 6-15 8-17 12-13  
exact bonds :  
3-4 3-8 4-5 5-6 6-7 7-8 7-10 7-16 10-11 11-12 12-18  
isolated ring systems :  
containing 3 :

G1

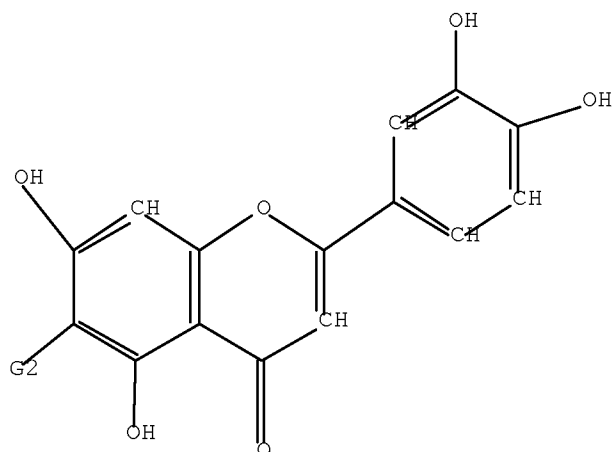
G2:H, MeO

G3

Connectivity :  
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:1 E exact RC ring/chain  
17:1 E exact RC ring/chain  
Match level :  
3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:CLASS

12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

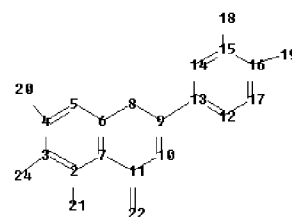
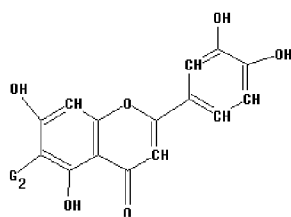
L40 STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L40.str



chain nodes :  
18 19 20 21 22 24  
ring nodes :  
2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17  
chain bonds :  
2-21 3-24 4-20 9-13 11-22 15-18 16-19  
ring bonds :  
2-3 2-7 3-4 4-5 5-6 6-7 6-8 7-11 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17  
exact/norm bonds :

2-21 3-24 4-20 11-22 15-18 16-19

exact bonds :

6-8 7-11 8-9 9-10 9-13 10-11

normalized bonds :

2-3 2-7 3-4 4-5 5-6 6-7 12-13 12-17 13-14 14-15 15-16 16-17

isolated ring systems :

containing 2 : 12 :

G1

G2:H, MeO

G3

Match level :

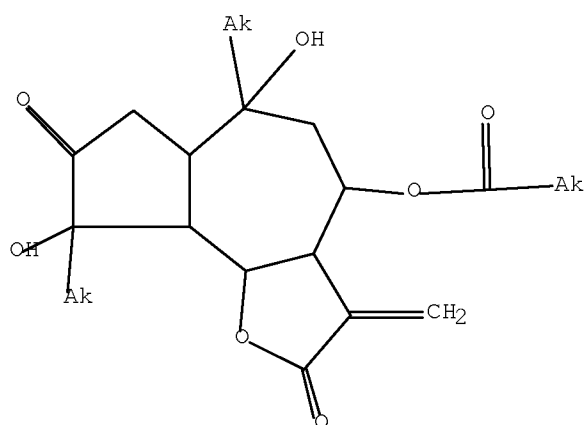
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12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS

21:CLASS 22:CLASS 24:CLASS

L41

STR



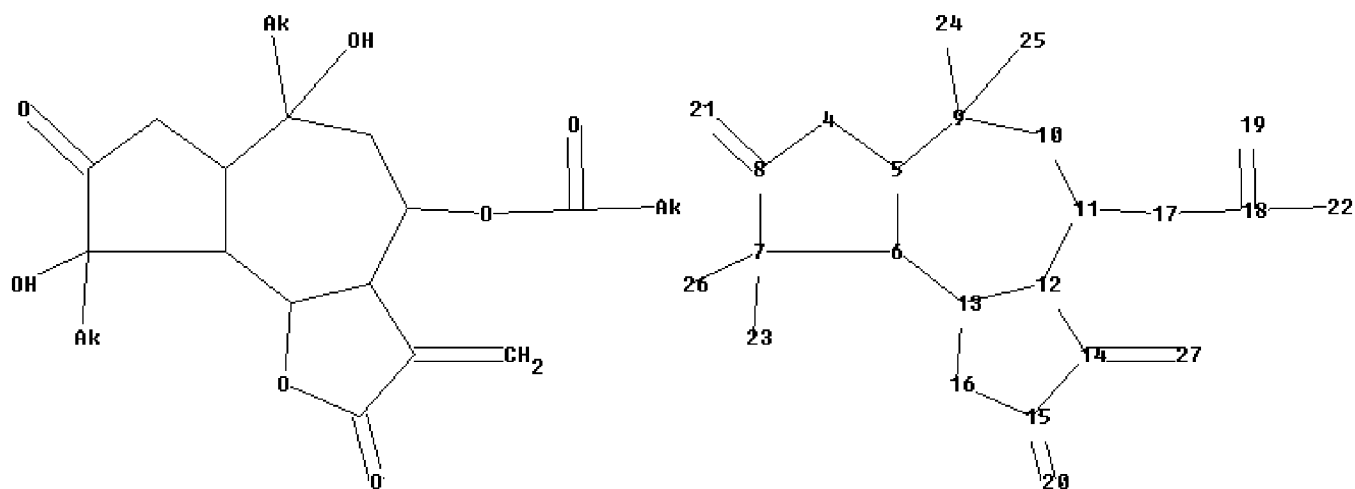
G1

G2 H, MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L41.str



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chain nodes :
17 18 19 20 21 22 23 24 25 26 27
ring nodes :
4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
7-23 7-26 8-21 9-24 9-25 11-17 14-27 15-20 17-18 18-19 18-22
ring bonds :
4-5 4-8 5-6 5-9 6-7 6-13 7-8 9-10 10-11 11-12 12-13 12-14 13-16 14-15
15-16
exact/norm bonds :
7-23 8-21 9-24 11-17 15-20 17-18 18-19 18-22
exact bonds :
4-5 4-8 5-6 5-9 6-7 6-13 7-8 7-26 9-10 9-25 10-11 11-12 12-13 12-14
13-16 14-15 14-27 15-16
isolated ring systems :
containing 4 :

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G1

G2:H, MeO

G3

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Connectivity :
22:1 E exact RC ring/chain 23:1E exact RC ring/chain 24:1 E exact RC ring/chain
Match level :
4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS

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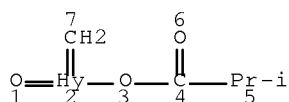
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              L39 OR L40 OR L41)

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L46          STR

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NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS PCY AT 2  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE  
 L49 10 SEA FILE=REGISTRY SUB=L44 SSS FUL L46

100.0% PROCESSED 15 ITERATIONS 10 ANSWERS  
 SEARCH TIME: 00.00.01 =FORMULAS I, II, IV, V, VI, IX

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 L35 STR  
 L36 STR  
 L37 STR  
 L38 STR  
 L39 STR  
 L40 STR  
 L41 STR  
 L44 65 SEA FILE=REGISTRY SUB=L8 SSS FUL (L35 OR L36 OR L37 OR L38 OR  
 L39 OR L40 OR L41)  
 L51 328280 SEA FILE=REGISTRY ABB=ON 3S  
 L53 1 SEA FILE=REGISTRY ABB=ON L51 AND L44 AND 1/NR =FORMULA III

L5 STR  
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 L35 STR  
 L36 STR  
 L37 STR  
 L38 STR  
 L39 STR  
 L40 STR  
 L41 STR  
 L44 65 SEA FILE=REGISTRY SUB=L8 SSS FUL (L35 OR L36 OR L37 OR L38 OR  
 L39 OR L40 OR L41)  
 L50 30 SEA FILE=REGISTRY ABB=ON L44 AND BENZOPYRAN  
 L54 26 SEA FILE=REGISTRY ABB=ON L50 AND 1/NC  
 L59 12 SEA FILE=REGISTRY ABB=ON L50 AND (6-7/O)  
 L60 8 SEA FILE=REGISTRY ABB=ON L59 AND L54  
 L62 2 SEA FILE=REGISTRY ABB=ON L59 AND (MONOHYDRATE OR SODIUM)  
 L63 10 SEA FILE=REGISTRY ABB=ON (L60 OR L62) =FORMULA VII, VIII

=> fil capl; d que nos 174  
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L5          STR
L8          237 SEA FILE=REGISTRY SSS FUL L5
L35         STR
L36         STR
L37         STR
L38         STR
L39         STR
L40         STR
L41         STR
L44         65 SEA FILE=REGISTRY SUB=L8 SSS FUL (L35 OR L36 OR L37 OR L38 OR
           L39 OR L40 OR L41)
L46         STR
L49         10 SEA FILE=REGISTRY SUB=L44 SSS FUL L46
L50         30 SEA FILE=REGISTRY ABB=ON L44 AND BENZOPYRAN
L51         328280 SEA FILE=REGISTRY ABB=ON 3S
L53         1 SEA FILE=REGISTRY ABB=ON L51 AND L44 AND 1/NR
L54         26 SEA FILE=REGISTRY ABB=ON L50 AND 1/NC
L59         12 SEA FILE=REGISTRY ABB=ON L50 AND (6-7/O)
L60         8 SEA FILE=REGISTRY ABB=ON L59 AND L54
L62         2 SEA FILE=REGISTRY ABB=ON L59 AND (MONOHYDRATE OR SODIUM)
L63         10 SEA FILE=REGISTRY ABB=ON (L60 OR L62)
L64         4165 SEA FILE=CAPLUS ABB=ON L63
L65         449 SEA FILE=CAPLUS ABB=ON L63/P
L66         395075 SEA FILE=CAPLUS ABB=ON CHROMATOG?/OBI
L67         22 SEA FILE=CAPLUS ABB=ON L65 AND L66
L68         50 SEA FILE=CAPLUS ABB=ON (L53 OR L49)
L69         50 SEA FILE=CAPLUS ABB=ON L68 OR (L68 AND L64)
L70         184654 SEA FILE=CAPLUS ABB=ON ANTITUMOR AGENTS/CT
L71         482074 SEA FILE=CAPLUS ABB=ON NEOPLAS?/CW
L72         28 SEA FILE=CAPLUS ABB=ON L65 AND (L70 OR L71)
L73         98 SEA FILE=CAPLUS ABB=ON (L67 OR L69 OR L72)
L74         64 SEA FILE=CAPLUS ABB=ON L73 AND (PY<2004 OR AY<2004 OR
           PRY<2004)

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=> s 174 not 119

L75 63 L74 NOT L19 L19=INVENTOR SEARCH ANSWER SET

=> d ibib abs hitstr 1-63; fil hom

L75 ANSWER 1 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:428226 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 142:451717  
 TITLE: Compositions containing herbal medicine components, emulsifiers, and diacylglycerols for increased absorption and manufacture thereof  
 INVENTOR(S): Oki, Kiyotoshi  
 PATENT ASSIGNEE(S): Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005126414	A	20050519	JP 2004-252417	20040831 <--
US 2006045928	A1	20060302	US 2005-152403	20050614
CN 1742983	A	20060308	CN 2005-10080739	20050630

PRIORITY APPLN. INFO.: JP 2003-319356 A 20030911 <--  
 JP 2004-252417 A 20040831

AB Compns., which show increased absorption of fat-soluble components from small intestine, are manufactured by letting mixts. of diacylglycerols with emulsifiers contain herbal medicine components. Thus, a composition prepared by heating 100 g diacylglycerol with 5 g lecithin and 1 g tetrahydrocurcumin was made into soft capsules.

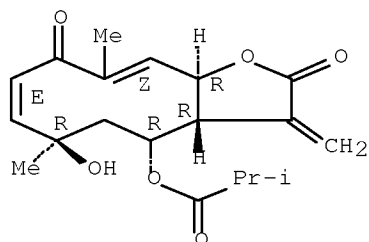
IT 59979-56-5, Tagitinin C  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (compns. containing herbal medicine components, emulsifiers, and diacylglycerols for increased absorption of fat-soluble components)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

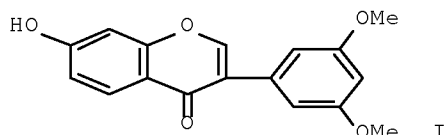
Absolute stereochemistry.

Double bond geometry as described by E or Z.

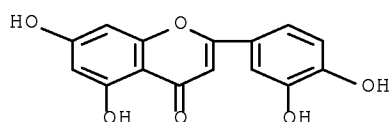


L75 ANSWER 2 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:174291 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 141:239805  
 TITLE: A New Isoflavone from Astragalus peregrinus  
 AUTHOR(S): Abd El-Latif, R. R.; Shabana, M. H.; El-Gandour, A. H.; Mansour, R. M.; Sharaf, M.

CORPORATE SOURCE: Phytochemistry and Plant Systematic Department,  
National Research Centre, Dokki, Cairo, 12311, Egypt  
SOURCE: Chemistry of Natural Compounds (Translation of Khimiya  
Prirodnikh Soedinenii) (2003), 39(6),  
536-537  
CODEN: CHNCA8; ISSN: 0009-3130  
PUBLISHER: Kluwer Academic/Consultants Bureau  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB In addition to daidzein, genistein, luteolin, apigenin, and apigenin-7-O-neohesperidoside, the methanol extract of the aerial parts of *Astragalus peregrinus* yielded a new isoflavone identified as 7-hydroxy-3',5'-dimethoxyisoflavone (I).  
IT 491-70-3P, Luteolin  
RL: BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)  
(new isoflavone from *Astragalus peregrinus*)  
RN 491-70-3 CAPLUS  
CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)

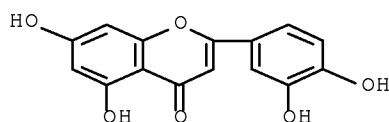


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 3 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2004:14709 CAPLUS Full-text  
DOCUMENT NUMBER: 141:20384  
TITLE: Chemical constituents of *Pterocaulon redolens*  
AUTHOR(S): Kanlayavattanakul, Mayuree; Ruangrunsi, Nijisiri; Watanabe, Toshiko; Ishikawa, Tsutomu  
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok, 10330, Thailand  
SOURCE: Heterocycles (2003), 61, 183-187  
CODEN: HTCYAM; ISSN: 0385-5414  
PUBLISHER: Japan Institute of Heterocyclic Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Studies on the chemical constituents of the aerial parts of *Pterocaulon redolens* (Forst.f) F. Vill. (Asteraceae) resulted in the isolation of ten

components: seven coumarins [5-methoxy-6,7-methylenedioxy coumarin (1), ayapin (2), puberulin (3), 5-methoxyscopoletin (4), 2',3'- dihydroxypuberulin (5), isofraxidin (6), and 5-(2',3'-dihydroxy-3'- methylbutyloxy)-6, 7-methylenedioxy coumarin (7)] and three flavonoids [luteolin (8), tomentin (9), and chrysosplenol C (10)], among which 5 was firstly isolated as a natural product. The full <sup>1</sup>H- and <sup>13</sup>C-NMR spectral assignments for the isolated products, including revision of previous assignment in the literature are reported. Six coumarins (1-4, 6, and 7) and one flavonoid (8) displayed mild activity against *Mycobacterium tuberculosis* H37Ra. In addition, flavonoid (10) was firstly found to possess moderate cytotoxicity against breast cancer (BC) and human small cell lung cancer (NCI-H187) cell lines.

IT 491-70-3P, Luteolin  
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);  
 PRP (Properties); PUR (Purification or recovery); BIOL (Biological study);  
 PREP (Preparation)  
 (chemical constituents of *Pterocaulon redolens*)  
 RN 491-70-3 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



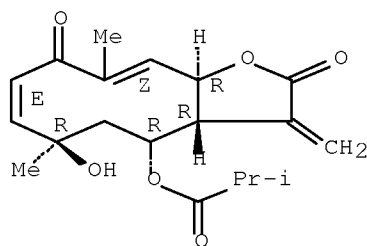
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 4 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:963428 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 141:35693  
 TITLE: Quantification of tagitinin C in *Tithonia diversifolia* by reversed-phase high-performance liquid chromatography  
 AUTHOR(S): Goffin, Eric; Proenca Da Cunha, Antonio; Ziemons, Eric; Tits, Monique; Angenot, Luc; Frederich, Michel  
 CORPORATE SOURCE: Laboratory of Pharmacognosy and Structural Chemistry, Natural and Synthetic Drugs Research Centre, University of Liege, Liege, Belg.  
 SOURCE: Phytochemical Analysis (2003), 14(6), 378-380  
 CODEN: PHANEL; ISSN: 0958-0344  
 PUBLISHER: John Wiley & Sons Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A simple, rapid and reliable reversed-phase high-performance liquid chromatog. method for the determination of tagitinin C, an anti-plasmodial sesquiterpene lactone isolated from the aerial parts of *Tithonia diversifolia*, has been developed. The assay has been used to quantify tagitinin C in various exts. of the aerial parts of *T. diversifolia*.

IT 59979-56-5, Tagitinin C  
 RL: ANT (Analyte); ANST (Analytical study)  
 (tagitinin C determination in *Tithonia diversifolia* by reversed-phase HPLC)  
 RN 59979-56-5 CAPLUS  
 CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as described by E or Z.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 5 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:835805 CAPLUS Full-text

DOCUMENT NUMBER: 140:192416

TITLE: Specific inhibition of hypoxia-inducible factor (HIF)-1 $\alpha$  activation and of vascular endothelial growth factor (VEGF) production by flavonoids

AUTHOR(S): Hasebe, Yuki; Egawa, Kiyoshi; Yamazaki, Yoko; Kunitomo, Setsuko; Hirai, Yasuaki; Ida, Yoshiteru; Nose, Kiyoshi

CORPORATE SOURCE: Department of Microbiology, Showa University School of Pharmaceutical Sciences, Tokyo, 142-8555, Japan

SOURCE: Biological & Pharmaceutical Bulletin (2003), 26(10), 1379-1383

CODEN: BPBLEO; ISSN: 0918-6158

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

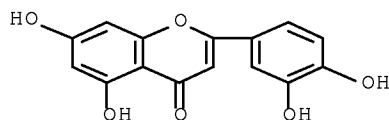
AB Screening using a reporter under the control of the hypoxia-response element (HRE) identified several flavonoids and homoisoflavonoids that inhibit the activation of HRE under hypoxic conditions. Among various compds., isorhamnetin, luteolin, quercetin, and Me ophiopogonanone B (MOB) were effective at 3 to 9  $\mu$ g/mL in inhibiting the reporter activity. The expression of vascular endothelial growth factor (VEGF) mRNA during hypoxia was also inhibited by MOB in HepG2 cells, but the EDs were 10 to 20  $\mu$ g/mL. MOB caused destabilization of hypoxia-inducible factor (HIF)-1 $\alpha$ , as revealed by Western blotting, that was dependent on proteasome activity and the tumor suppressor, p53. The tubular formation and migration of human umbilical vein endothelial cells was also inhibited by MOB. MOB is expected to act as an inhibitor of angiogenesis.

IT 491-70-3P, Luteolin

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)  
(inhibition of HIF-1 $\alpha$  VEGF production by flavonoids)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



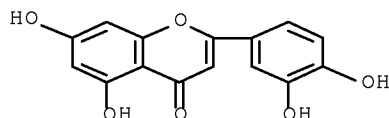
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L75 ANSWER 6 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:234903 CAPLUS Full-text  
 DOCUMENT NUMBER: 139:94966  
 TITLE: Inhibitory effects of luteolin isolated from Ixeris sonchifolia Hance on the proliferation of HepG2 human hepatocellular carcinoma cells  
 AUTHOR(S): Yee, Su Bog; Lee, Jung Hwa; Chung, Hae Young; Im, Kwang Sik; Bae, Song Ja; Choi, Jae Soo; Kim, Nam Deuk  
 CORPORATE SOURCE: Department of Pharmacy, Pusan National University, Pusan, 609-735, S. Korea  
 SOURCE: Archives of Pharmacal Research (2003), 26(2), 151-156  
 CODEN: APHRDQ; ISSN: 0253-6269  
 PUBLISHER: Pharmaceutical Society of Korea  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB We investigated the anti-proliferative effects of luteolin and apigenin, isolated from Ixeris sonchifolia Hance, on HepG2 human hepatocellular carcinoma cells. In MTT assay luteolin showed more efficient anti-proliferative effects on cells than apigenin did. According to propidium iodide staining and flow cytometry studies, we postulated that these effects might be a result of cell cycle arrest. Hence we examined the changes of protein expressions related to cell cycle arrest. Western blotting data demonstrated that the down-regulated expression of CDK4 was correlated to the increase of p53 and CDK inhibitor p21WAF1/CIP1 protein. These data suggest that luteolin may have potential as an anti-cancer agent.

IT 491-70-3P, Luteolin  
 RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (inhibitory effects of luteolin isolated from Ixeris sonchifolia on proliferation of HepG2 human hepatocellular carcinoma cells)

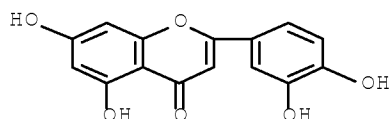
RN 491-70-3 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

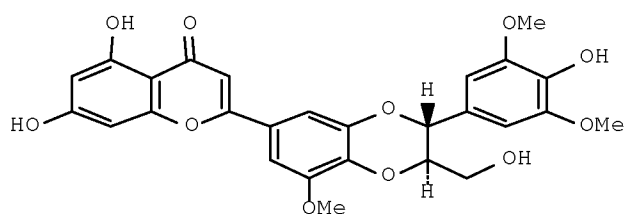
L75 ANSWER 7 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:169133 CAPLUS Full-text

DOCUMENT NUMBER: 139:257475  
 TITLE: Optimization of HPLC separations of flavonoids with the use of artificial neural networks  
 AUTHOR(S): Bucinski, Adam; Baczek, Tomasz  
 CORPORATE SOURCE: Institute of Animal Reproduction and Food Research, Division of Food Science, Polish Academy of Sciences, Olsztyn, Pol.  
 SOURCE: Polish Journal of Food and Nutrition Sciences ( 2002), 11(4), 47-51  
 CODEN: PJFSE7; ISSN: 1230-0322  
 PUBLISHER: Polish Academy of Sciences, Institute of Animal Reproduction and Food Research, Division of Food Science  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The high-performance liquid chromatog. (HPLC) procedure based on gradient elution technique was used to sep. flavonoids in leaves of *Taxus baccata* var *elegantissima* and *Metasequoia glyptostroboides*. Optimization of chromatog. sepns. was supported by artificial neural networks. The best gradient conditions acquired to sep. analyzed compds. were established and then used in expts. Predictive errors were addnl. calculated Satisfactory correlation between predicted and exptl. retention data was obtained.  
 IT 491-70-3P, Luteolin  
 RL: PUR (Purification or recovery); PREP (Preparation)  
 (optimization of HPLC sepns. of flavonoids from plant leaf with use of artificial neural networks)  
 RN 491-70-3 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 8 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:67364 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 138:268406  
 TITLE: Isolation and structure of palstatin from the Amazon tree *Hymenaea palustris*  
 AUTHOR(S): Pettit, George R.; Meng, Yanhui; Stevenson, Clare A.; Doubek, Dennis L.; Knight, John C.; Cichacz, Zbigniew; Pettit, Robin K.; Chapuis, Jean-Charles; Schmidt, Jean M.  
 CORPORATE SOURCE: Cancer Research Institute and Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, 85287-2404, USA  
 SOURCE: Journal of Natural Products (2003), 66(2), 259-262  
 CODEN: JNPRDF; ISSN: 0163-3864  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



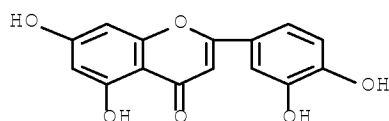
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AB Bioassay (P388 lymphocytic leukemia cell line and human cancer cell lines)-guided separation of an extract prepared from the leaves of *Hymenaea palustris* Ducke led to the isolation of six cancer cell growth inhibitory flavonoids (1-6). The structures were elucidated by HRMS and 1D and 2D NMR spectral anal. The new flavonolignan I, designated palstatin, proved to be a methoxy structural modification of 5'-methoxyhydnocarpin-D (2). Flavones 1-4 inhibited growth of the pathogenic bacteria *Enterococcus faecalis* and/or *Neisseria gonorrhoeae*.

IT 491-70-3F, Luteolin  
 RL: BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation) (isolation and structure of palstatin and other flavonoids from Amazon tree *palustris*)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 9 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:966926 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:57728

TITLE: Analysis of flavonoids in *Vernonia paltula* by high-performance liquid chromatography

AUTHOR(S): Ku, Yoe-Ray; Chen, Chi-Yuan; Ho, Li-Kang; Lini, Jer-Huei; Chang, Yuan-Shiun

CORPORATE SOURCE: Department of Health, National Laboratories of Foods and Drugs, Nankang, Taipei, 115, Taiwan

SOURCE: Yaowu Shipin Fenxi (2002), 10(3), 139-142  
 CODEN: YSFEEP; ISSN: 1021-9498

PUBLISHER: National Laboratories of Food and Drugs, Dep. of Health, Executive Yuan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Lin-nan-yeh-chu, is the dried entire plant of *Vernonia paltula* (Compositae) and used as folk medicine in Taiwan. To evaluate the quality of *V. paltula*, a simple, rapid, and accurate high-performance liquid chromatog. (HPLC) method

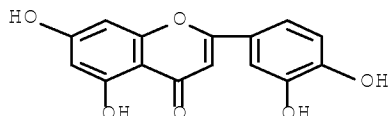
was developed for the assay of 4 flavonoids apigenin (API), apigenin-7-O-glucoside (APG), luteolin (LUT), and luteolin-7-O-glucoside (LUG). The present HPLC system uses an Inertsil ODS-2 column by gradient elution with acetonitrile and 0.1% (volume/volume) phosphoric acid as the mobile phase. Et paraben was used as an internal standard and detected at 254 nm. Regression equations revealed good linear relationships (correlation coeffs.: 0.9998-0.9999) between the peak-area ratios of each constituent to Et paraben. The recovery of 4 marker constituents ranged from 89.3 to 95.6%. The contents of the 4 constituents in stem, flower, leaf, and root parts of *V. paltula* were compared. Leaf part consisted of the highest contents of flavonoids except for APG which is less than that in the flower. The root and stem only showed trace amount of APG but not the other 3 flavonoids. The contents of 4 constituents were 0.6016, 0.0042, 0.2160, and 0.0577 mg/g for apigenin-7-O-glucoside, apigenin, luteolin-7-O-glucoside and luteolin, resp. HPLC chromatograms of another 3 plants of genus of *Vernonia* in Taiwan, *V. cinerea*, *V. elliptica* and *V. gratiola*, were also compared.

IT 491-70-3P, Luteolin

RL: PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(anal. of flavonoids in *Vernonia paltula* by HPLC)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 10 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:669877 CAPLUS Full-text

DOCUMENT NUMBER: 137:345604

TITLE: Antiproliferative Activities of Citrus Flavonoids against Six Human Cancer Cell Lines

AUTHOR(S): Manthey, John A.; Guthrie, Najla

CORPORATE SOURCE: U.S. Citrus and Subtropical Products Laboratory, South Atlantic Area Agricultural Research Service, U.S. Department of Agriculture, Winter Haven, FL, 33881, USA

SOURCE: Journal of Agricultural and Food Chemistry (2002), 50(21), 5837-5843  
CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:345604

AB Citrus fruits contain high concns. of several classes of phenols, including numerous hydroxycinnamates, flavonoid glycosides, and polymethoxylated flavones. The latter group of compds. occurs without glycosidic linkages and has been shown to inhibit the proliferation of a number of cancer cell lines. This antiproliferative property was further demonstrated against addnl. human cancer cell lines, and the antiproliferative actions of a series of synthetic methoxylated flavones were also studied. Similar to the naturally occurring compds., the synthetic compds. exhibited strong antiproliferative activities.

In many cases the IC<sub>50</sub> values occurred below 10  $\mu$ m. Other hydroxylated flavone and flavanone aglycons also exhibited antiproliferative activities against the cancer cell lines, with the flavones showing greater activities than the flavanones. Glycosylation of these compds. removed their activity. The strong antiproliferative activities of the polymethoxylated flavones suggest that they may have use as anticancer agents in humans.

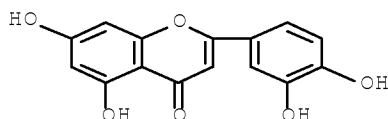
IT 491-70-3F, Luteolin

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antiproliferative activities of Citrus flavonoids against six human cancer cell lines)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 11 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:625520 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 138:163104

TITLE: Cytotoxicity of phenolic compounds isolated from seeds of safflower (*Carthamus tinctorius* L.) on cancer cell lines

AUTHOR(S): Bae, Song-Ja; Shim, Sun-Mi; Park, Yun-Ja; Lee, Jun-Young; Chang, Eun-Ju; Choi, Sang-Won

CORPORATE SOURCE: Department of Food Science and Nutrition, Catholic University of Daegu, Hayang, Gyeongbuk, 712-702, S. Korea

SOURCE: Food Science and Biotechnology (2002), 11(2), 140-146

CODEN: FSB0BR; ISSN: 1226-7708

PUBLISHER: Korean Society of Food Science and Technology

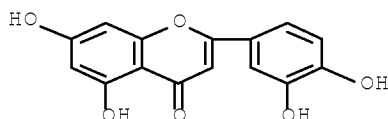
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The methanolic extract of roasted safflower seeds exhibited moderate cytotoxicity against three cancer cell lines, HepG2, MCF-7, and HeLa, in a dose-dependent manner, as measured by MTT assay. The methanolic extract was further partitioned with n-hexane, Et acetate and n-butanol successively. The Et acetate fraction exhibited potent cytotoxicities against the cancer cell lines. N-Feruloylserotonin (S1), N-(p-coumaroyl)serotonin (S2), matairesinol (L1), 8'-hydroxyarctigenin (L2), luteolin (F1), and acacetin (F2) were isolated from the Et acetate extract, and their chemical structures were identified by UV, IR, NMR, and MS spectroscopic methods. Six phenolic compds. possessed comparable cytotoxicity against three cancer cells. In particular, F1 and F2 had the most potent cytotoxicity with IC<sub>50</sub> values of 51.8 and 62.1  $\mu$ g/mL for HeLa cell, 33.6 and 37.7  $\mu$ g/mL for MCF-7 cell and 47.3 and 56.6  $\mu$ g/mL for HepG2 cell, resp. In addition, L1, L2, S1, and S2 also showed strong cytotoxicity, although activities of serotoninins were weaker than those of lignans. On normal human liver cell (WRL68) at a high concentration of 100

µg/mL, two serotoninins and lignans did not show any cytotoxicity, and two flavonoids exhibited only about 50% cytotoxicity. These results suggest that phenolic compds. in the safflower seeds may be useful as potential cancer chemopreventive agents.

IT 491-70-3P, Luteolin  
 RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (cytotoxicity of phenolic compds. isolated from seeds of safflower (*Carthamus tinctorius*) on cancer cell lines)  
 RN 491-70-3 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 12 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:549130 CAPLUS Full-text

DOCUMENT NUMBER: 137:221861

TITLE: In vitro antiplasmodial activity of *Tithonia diversifolia* and identification of its main active constituent: Tagitinin C

AUTHOR(S): Goffin, Eric; Ziemons, Eric; De Mol, Patrick; de Ceudeville, Maria; Martins, Ana Paula; Proenca da Cunha, Antonio; Philippe, Genevieve; Tits, Monique; Angenot, Luc; Frederich, Michel

CORPORATE SOURCE: Laboratory of Pharmacognosy, Natural and Synthetic Drugs Research Center, University of Liege, Liege, B-4000, Belg.

SOURCE: *Planta Medica* (2002), 68(6), 543-545

CODEN: PLMEAA; ISSN: 0032-0943

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The antimalarial properties of *Tithonia diversifolia*, an Asteraceae traditionally used to treat malaria, were investigated in vitro against 3 strains of *Plasmodium falciparum*. The ether extract from aerial parts of the plant collected in Sao Tome e Principe, demonstrated good antiplasmodial activity (IC<sub>50</sub> on FCA strain: 0.75 µg/mL). A bioassay guided fractionation of this extract led to the isolation of the known sesquiterpene lactone tagitinin C as an active component against *Plasmodium* (IC<sub>50</sub> on FCA strain: 0.33 µg/mL), but also possessing cytotoxic properties (IC<sub>50</sub> on HTC-116 cells: 0.706 µg/mL).

IT 59979-56-5P, Tagitinin C  
 RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)

(antiplasmodial and cytotoxic activity tagitinin C)

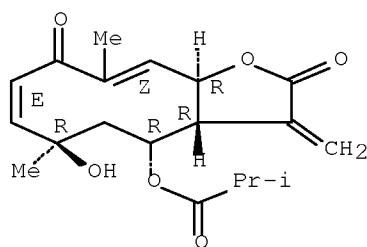
RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-

yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 13 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:303071 CAPLUS Full-text

DOCUMENT NUMBER: 138:149691

TITLE: OPLC and AMD, recent techniques of planar chromatography: their interest for separation and characterization of extractive and synthetic compounds

AUTHOR(S): Galand, N.; Pothier, J.; Dollet, J.; Viel, C.

CORPORATE SOURCE: Faculte de Pharmacie 'Philippe Maupas', Laboratoire de Pharmacognosie, Tours, 37200, Fr.

SOURCE: Fitoterapia (2002), 73(2), 121-134  
CODEN: FTRPAE; ISSN: 0367-326X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB It is always important for the chemist to have good methods of separation, characterization and quant. evaluation for one or several compds. resulting from a chemical reaction or an extraction procedure. In this domain the chromatog. techniques are choice methods, in particular Over Pressured Layer Chromatog. (OPLC) and Automated Multiple Development (AMD). They are relatively recent methods whose use is unfortunately not yet generalized although they give very clean separation. In this paper we present numerous examples of the use of these two new types of planar chromatogs. and especially the results we have obtained in the field of natural products on a wide variety of different structures: coumarins, flavonoids, anthocyanins, alkaloids and essential oils.

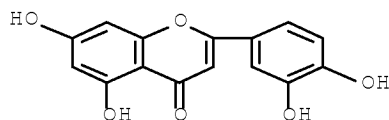
IT 491-70-3P, Luteolin

RL: ANT (Analyte); PUR (Purification or recovery); ANST (Analytical study); PREP (Preparation)

(separation and characterization of natural products and synthetic compds. by overpressured thin-layer chromatog. and automated multiple development)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 14 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:221323 CAPLUS Full-text  
 DOCUMENT NUMBER: 136:398536  
 TITLE: Sesquiterpenoids from *Tithonia diversifolia* with potential cancer chemopreventive activity  
 AUTHOR(S): Gu, Jian-Qiao; Gills, Joell J.; Park, Eun Jung; Mata-Greenwood, Eugenia; Hawthorne, Michael E.; Axelrod, Franklin; Chavez, Pedro I.; Fong, Harry H. S.; Mehta, Rajendra G.; Pezzuto, John M.; Kinghorn, A. Douglas  
 CORPORATE SOURCE: Program for Collaborative Research in the Pharmaceutical Sciences and Department of Medicinal Chemistry and Pharmacognosy College of Pharmacy, University of Illinois at Chicago, Chicago, IL, 60612, USA  
 SOURCE: Journal of Natural Products (2002), 65(4), 532-536  
 CODEN: JNPRDF; ISSN: 0163-3864  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Activity-guided fractionation of an Et acetate extract of the aerial parts of *Tithonia diversifolia*, using an antiproliferation bioassay performed with human colon cancer (Col2) cells, led to the isolation of three new sesquiterpenoids, 2 $\alpha$ -hydroxytirotundin (I), tithofolinolide (II), and 3 $\alpha$ -acetoxyldiversifolol (III), along with eight known sesquiterpene lactones, 3 $\beta$ -acetoxyl-8 $\beta$ -isobutyryloxyreynosin (IV), tagitinin C (V), 1 $\beta$ ,2 $\alpha$ -epoxytagitinin C (VI), 4 $\alpha$ ,10 $\alpha$ -dihydroxy-3-oxo-8 $\beta$ -isobutyryloxyguaia-11(13)-en- 12,6 $\alpha$ -olide (VII), 3 $\alpha$ -acetoxyl-4 $\alpha$ -hydroxy-11(13)-eudesmen- 12-oic acid Me ester, 17,20-dihydroxygeranylnerol, tagitinin A, and tirotundin. These isolates were evaluated for their potential as cancer chemopreventive agents, by measuring antiproliferative activity in Col2 cells and induction of cellular differentiation in human promyelocytic leukemia (HL-60) cells. Selected compds. were then investigated for their ability to inhibit 7,12-dimethylbenz[*a*]anthracene-induced preneoplastic lesions in a mouse mammary organ culture assay. Among these isolates, V and VI showed significant antiproliferative activity, II, IV, and VII induced HL-60 cellular differentiation, and IV significantly inhibited (63.0% at 10  $\mu$ g/mL) lesion formation in the mouse mammary organ culture assay. The chemical structures of I-III were elucidated by spectroscopic anal. The absolute configurations of I and II were determined by Mosher ester methodol.

IT 59979-56-5, Tagitinin C 110382-30-4,

4 $\alpha$ ,10 $\alpha$ -Dihydroxy-3-oxo-8 $\beta$ -isobutyryloxyguaia-11(13)-en-  
12,6 $\alpha$ -olide

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);

BIOL (Biological study)

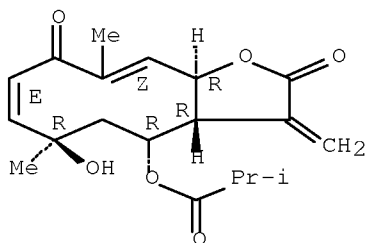
(from *Tithonia diversifolia* with potential cancer chemopreventive activity)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

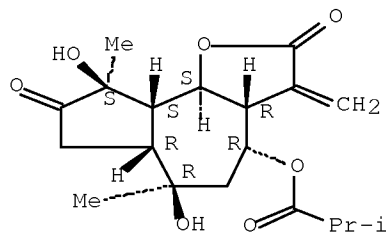
Double bond geometry as described by E or Z.



RN 110382-30-4 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,6aR,9S,9aS,9bS)-dodecahydro-6,9-dihydroxy-6,9-dimethyl-3-methylene-2,8-dioxoazuleno[4,5-b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 15 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:146758 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 137:166169

TITLE: Cytotoxic principles from the leaves of *Tithonia diversifolia*

AUTHOR(S): Wu, Tian-Shung; Shi, Li-Shian; Kuo, Ping-Chung; Leu, Yann-Lii; Liou, Meei-Jen; Wu, Pei-Lin; Wu, Yang-Chang; Iou, Song-Chou; Chen, Yuh-Pan; Chang, Hsien-Chang

CORPORATE SOURCE: Department of Chemistry, National Cheng Kung University, Tainan, 701, Taiwan

SOURCE: Chinese Pharmaceutical Journal (Taipei, Taiwan) (2001), 53(5), 217-223

CODEN: CPHJEP; ISSN: 1016-1015

PUBLISHER: Pharmaceutical Society of Republic of China  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Three compds., acetyltagitinin E, tagitinin-F and hispidulin, were isolated from the leaves of *Tithonia diversifolia*. The stereochem. of acetyltagitinin E was further supported by X-ray crystallog. The cytotoxicity of these compds. was also determined. Compds. acetyltagitinin E and tagitinin-F showed selective cytotoxicity to Hep G2 human hepatocellular carcinoma cells.

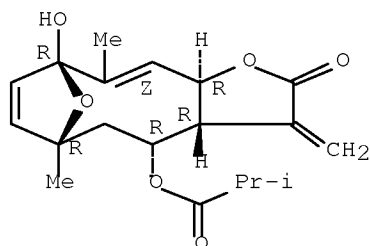
IT 59979-57-6P, Tagitinin-F  
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (from the leaves of *Tithonia diversifolia*)

RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 16 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:463926 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:193641

TITLE: Isolation and cytotoxicity of flavonoids from *Daphnis Genkwa* Flos

AUTHOR(S): Lin, Jer-Huei; Lin, Ya-Tze; Huang, Yuh-Jan; Wen, Kuo-Ching; Chen, Ruei-Ming; Ueng, Tzue-Huei; Liao, Chun-Heng

CORPORATE SOURCE: Taipei, National Laboratories of Foods and Drugs, Taiwan

SOURCE: Yaowu Shipin Fenxi (2001), 9(1), 6-11

CODEN: YSFEEP; ISSN: 1021-9498

PUBLISHER: National Laboratories of Food and Drugs, Dep. of Health, Executive Yuan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB For the purpose of quality anal., we investigated polar constituents as marker substance for some traditional herbs. From *Daphnis Genkwa* Flos twelve flavonoids were isolated. They were identified as potassium apigenin 7-O- $\beta$ -D-glucuronate (1), apigenin 7-O- $\beta$ -D-glucuronide (2), apigenin 7-O- $\beta$ -D-methylglucuronate (3), apigenin (4), genkwanin 5-O- $\beta$ -D-primeveroside (5), genkwanin 5-O- $\beta$ -D-glucoside (6), genkwanin (7), tiliroside (8), kaempferol (9), luteolin 5-O- $\beta$ -D-glucoside (10), luteolin (11) and 7-O-methyluteolin (12). Among them, 2, 3, 5, 6, 9 and 10 were known compds., but were for the

first time isolated from this material. Compound 1 was isolated from nature for the first time. The structures of 1-12 were established on the basis of their phys. properties and spectroscopic evidence. Treatments of human hepatoma HepG2 cells with 0.1 mM apigenin, luteolin, and 7-O-methyluteolin for 48 h caused 40% reduction on cell viability, whereas potassium apigenin 7-O- $\beta$ -D-glucuronate, luteolin 5-O- $\beta$ -D-glucoside, genkwanin, genkwanin 5-O- $\beta$ -D-primeveroside, and tiliroside caused little or no effects on the viability of HepG2 cell. These data suggest a rough structure-activity relation of flavonoid cytotoxicity.

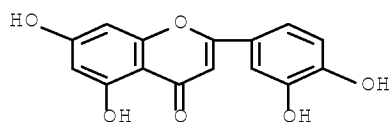
IT 491-70-3P, Luteolin

RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(isolation and antitumor structure activity relationships of flavonoids from *Daphnis Genkwae* Flos)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 17 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:704603 CAPLUS Full-text

DOCUMENT NUMBER: 134:97881

TITLE: Chemical constituent from *Tithonia diversifolia*

AUTHOR(S): Zhou, Hong; Peng, Liyan; Jiang, Bei; Hou, Aijun; Lin, Zhongwen; Sun, Handong

CORPORATE SOURCE: Laboratory of Phytochemistry, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming, 650204, Peop. Rep. China

SOURCE: Yunnan Zhiwu Yanjiu (2000), 22(3), 361-364, 370

CODEN: YCWCDP; ISSN: 0253-2700

PUBLISHER: Zhongguo Kexueyuan Kunming Zhiwu Yanjiuso

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The chemical constituents of *Tithonia diversifolia* were isolated and identified. Tagitinin A, tagitinin C, 3,5-di-O-caffeoylquinic acid were obtained.

IT 59979-56-5P, Tagitinin C

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

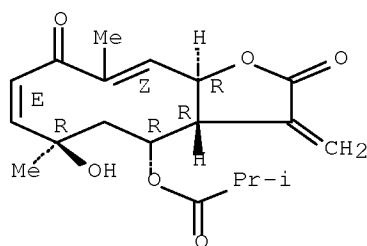
(constituents from *Tithonia diversifolia*)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

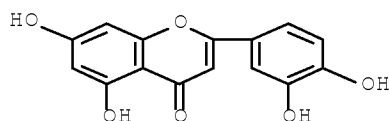
L75 ANSWER 18 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:408763 CAPLUS Full-text  
 DOCUMENT NUMBER: 131:240467  
 TITLE: Leaf surface flavonoids of Chrysothamnus  
 AUTHOR(S): Stevens, Jan F.; Wollenweber, Eckhard; Ivancic, Monika; Hsu, Victor L.; Sundberg, Scott; Deinzer, Max L.  
 CORPORATE SOURCE: Department of Chemistry, Oregon State University, Corvallis, OR, 97331, USA  
 SOURCE: Phytochemistry (1999), 51(6), 771-780  
 CODEN: PYTCAS; ISSN: 0031-9422  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Twenty-six flavonoid aglycons have been identified from eight plants covering three species of Chrysothamnus that were collected in eastern Oregon. The flavonoids were identified by NMR spectroscopy, tandem mass spectrometry and co-TLC with authentic markers. Chrysothamnus nauseosus yielded Me ethers of apigenin, isoscutellarein, luteolin, kaempferol, herbacetin and quercetin. O-Methylated kaempferol and quercetin derivs. were isolated from the leaf exudate of C. humilis. The flavonoid chemical of C. viscidiflorus was found different from the other two species by the presence of Me ethers of quercetin, eriodictyol and taxifolin-3-acetate. Although the flavonoid profiles proved of diagnostic value at the species level, they provided little further evidence in favor of inclusion of Chrysothamnus into Ericameria as proposed earlier on the basis of morphol. similarities.

IT 491-70-3P  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)  
 (isolation and characterization of leaf surface flavonoids of Chrysothamnus)

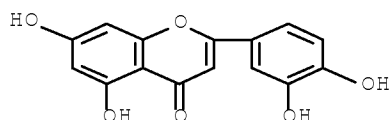
RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 19 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:400895 CAPLUS Full-text  
 DOCUMENT NUMBER: 131:197084  
 TITLE: Separation of flavonoids, coumarins, and anthocyanins in plant extracts by overpressured layer chromatography  
 AUTHOR(S): Galand, N.; Pothier, J.; Mason, V.; Viel, Claude  
 CORPORATE SOURCE: Laboratoire Pharmacochimie Produits Naturels Analogues Structuraux, Faculte Sciences Pharmaceutique, Univ. Tours, Tours, F-37200, Fr.  
 SOURCE: Pharmazie (1999), 54(6), 468-471  
 CODEN: PHARAT; ISSN: 0031-7144  
 PUBLISHER: Govi-Verlag Pharmazeutischer Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Flavonoids, coumarins, and anthocyanins were separated from plant exts. by overpressured layer chromatog. The best eluents were EtOAc/CHCl3 for flavonoids, coumarins, and furanochromones, and EtOAc/MeEtCO/HCOOH/HCl for anthocyanins.  
 IT 491-70-3P, Luteolin  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (flavonoids, coumarins, and anthocyanins in plant exts. separated by overpressured layer chromatog.)  
 RN 491-70-3 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

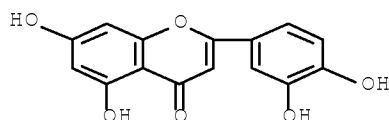
L75 ANSWER 20 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1998:394862 CAPLUS Full-text  
 DOCUMENT NUMBER: 129:120106  
 TITLE: Chemical constituents of Ixeris sonchifolia Hance  
 AUTHOR(S): Ma, Jiyuan; Wang, Zhengtao; Xu, Luoshan; Xu, Guojun; Wang, Yixian  
 CORPORATE SOURCE: Dep. Pharmacognosy, China Pharmaceutical Univ., Nanjing, 200038, Peop. Rep. China  
 SOURCE: Zhongguo Yaoke Daxue Xuebao (1998), 29(2), 94-96  
 CODEN: ZHYXE9; ISSN: 1000-5048  
 PUBLISHER: Zhongguo Yaoke Daxue  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese

AB Scopoletin, luteolin, apigenin, (E)-2,5-dihydroxycinnamic acid, bis-(2-ethylhexyl) phthalate, (+)-syringaresinol, p-hydroxybenzaldehyde, 1,4-benzenedimethanol were isolated from the herb of *Ixeris sonchifolia* Hance. The exts. of petroleum ether, chloroform, acetone and methanol from *I. sonchifolia* showed the inhibitory effect on murine ascites, hepatic and cervical carcinomas.

IT 491-70-3P, Luteolin  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses) (chemical constituents of *Ixeris sonchifolia* Hance)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



L75 ANSWER 21 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:478236 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 127:188212

TITLE: Sesquiterpene lactones from Brazilian *Tithonia diversifolia*

AUTHOR(S): Pereira, Paulo Sergio; Dias, Diones Aparecida; Vichnewski, Walter; Nasi, Ana Maria Turco Tucci; Herz, Werner

CORPORATE SOURCE: Departamento de Quimica, Faculdade de Filosofia, Ciencias e Letras de Ribeirao Preto, Universidad de Sao Paulo, Ribeirao Preto, 14040-901, Brazil

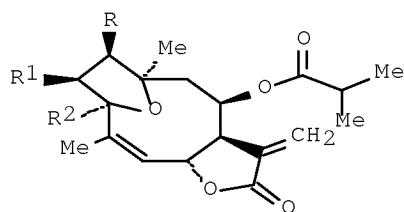
SOURCE: Phytochemistry (1997), 45(7), 1445-1448  
 CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I R=R2=OMe, R1=H  
 II R=H, R2=OMe, R3= OH

AB Aerial parts of *Tithonia diversifolia* collected in Sao Paulo State afforded two new heliangolides (I, II) in addition to the heliangolides tagitinin F and 1,2-epoxytagitinin C, one known guaianolide and the flavone hispidulin. Structures were established by spectroscopic studies.

IT 59979-57-6 110382-29-1

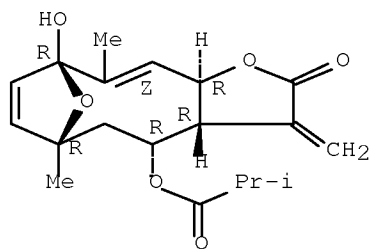
RL: BOC (Biological occurrence); BSU (Biological study, unclassified);  
 BIOL (Biological study); OCCU (Occurrence)  
 (sesquiterpene lactones from Brazilian *Tithonia diversifolia*)

RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

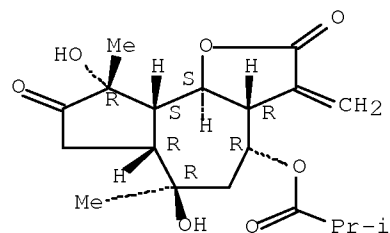
Double bond geometry as described by E or Z.



RN 110382-29-1 CAPLUS

CN Propanoic acid, 2-methyl-, dodecahydro-6,9-dihydroxy-6,9-dimethyl-3-methylene-2,8-dioxoazuleno[4,5-b]furan-4-yl ester, [3aR-(3aa, 4β, 6a, 6aa, 9β, 9aa, 9bβ)]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 22 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:179538 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 126:274753

TITLE: Characterization of flavonoids in extracts from four species of *Epimedium* by micellar electrokinetic capillary chromatography with diode-array detection

AUTHOR(S): Liang, H.-R.; Siren, H.; Jyske, P.; Reikkola, M.-L.; Vuorela, P.; Vuorela, H.; Hiltunen, R.

CORPORATE SOURCE: Lab. Analytical Chem., Univ. Helsinki, FIN-00014, Finland

SOURCE: Journal of Chromatographic Science (1997), 35(3), 117-125

CODEN: JCHSBZ; ISSN: 0021-9665

PUBLISHER: Preston Publications

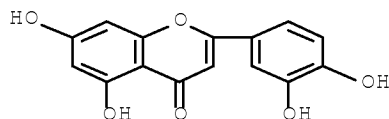
DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A micellar electrokinetic capillary chromatog. (MEKC) method with diode-array detection is developed for the characterization of pharmacol. active flavonoids in exts. prepared from *Epimedium brevicornum*, *E. humanense*, *E. coactum*, and *E. truncatum*. The pKa values of icariin, epimedin B, and epimedin C are determined by spectrophotometry. Optimal separation of icariin, epimedin B and C, and eight other compds. is achieved by determining pKa values and by systematically optimizing electrolytic and instrumental parameters. The repeatability of analyses and the reliability of identifications are evaluated by the marker technique. Calculated for relative migration times of flavonoids in the exts., the repeatability of the analyses varies from 0.7 to 6.4% (nine replicates). For migration indexes calculated with two markers, however, the repeatability almost falls below 0.5%. The distribution of the flavonoids is found to differ both qual. and quant. among the four species. The MEKC technique appears to provide a powerful tool for the identification and quality control of plant drugs and for phytotaxonomic investigations.

IT 491-70-3P, Luteolin  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (characterization of flavonoids in exts. from four species of *Epimedium* by micellar electrokinetic capillary chromatog. with diode-array detection)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



L75 ANSWER 23 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:417847 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 125:67741

TITLE: Flavones or anthocyanins as matrix metalloprotease inhibitors and their extraction from medicinal plants for therapeutic use

INVENTOR(S): Kumagai, Kazuo; Fujiwara, Fumi; Negoro, Takaatsu; Kaneoka, Shoji; Saji, Kitaro

PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

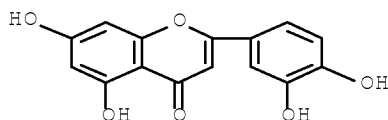
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08104628	A	19960423	JP 1994-266264	19941004 <--
PRIORITY APPLN. INFO.:			JP 1994-266264	19941004 <--
OTHER SOURCE(S):	MARPAT	125:67741		

AB Flavones or anthocyanins as matrix metalloprotease inhibitors and their extraction from medicinal plants (e.g. *Scutellaria baicalensis* roots) for therapeutic use are claimed. Baicalein inhibited the activity of matrix metalloprotease (e.g. collagenase) with  $IC_{50} = 25 \mu g/mL$ . The flavones or anthocyanins may be used for treating deformative arthropathy, gingivitis, cancer metastasis, and chronic rheumatism.

IT 491-70-3F, Luteolin  
 RL: PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (flavones or anthocyanins as matrix metalloprotease inhibitors and their extraction from plants for therapeutic use)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



L75 ANSWER 24 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:125154 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 124:219690

TITLE: Studies on cancer bio-chemoprevention of natural resources. X. Inhibitory effect of spices on TPA-enhanced 3H-choline incorporation in phospholipids of C3H10T1/2 cells and on TPA-induced mouse ear edema of C3H10T1/2 cells and on TPA-induced mouse ear edema

AUTHOR(S): Okuyama, Toru; Matsuda, Masayoshi; Masuda, Yuka; Baba, Masaki; Masubuchi, Harumi; Adachi, Megumi; Okada, Yoshihito; Hashimoto, Takao; Zou, Li-Bo; Nishino, Hoyoku

CORPORATE SOURCE: Department Phytochemistry and Pharmacognosy, Meiji College Pharmacy, Setagaya, 154, Japan

SOURCE: Chinese Pharmaceutical Journal (Taipei) (1995), 47(5), 421-30  
 CODEN: CPHJEP

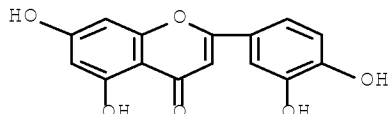
PUBLISHER: Pharmaceutical Society of Republic of China

DOCUMENT TYPE: Journal

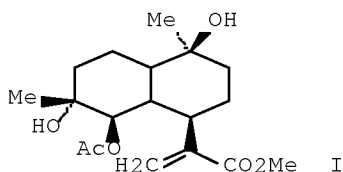
LANGUAGE: English

AB Thirty-seven kinds of spices were extracted with n-hexane, Et acetate and methanol to obtain the corresponding 111 exts. Each extract was examined for antitumor-promoting activity on 12-O-tetradecanoyl-phorbol-13-acetate (TPA)-enhanced 3H-choline incorporation into phospholipids of C3H10T1/2 cells in vitro and on TPA-induced mouse ear edema in vivo. Among the tested spices, Basil, Ginger, Marjoram, Rosemary, White Pepper and Xiebai significantly inhibited TPA-enhanced 3H-choline incorporation into phospholipids of C3H10T1/2 cells. Allspice, Basil, Bay (Laurel), Cardamom seed, Cinnamon, Cumin, Dill seed, Dry ginger, Ginger, Japanese parsley, Horse-radish, Marjoram, Oregano, Parsley, Pink pepper, Red pepper, Rosemary, Sage, Tarragon, Thyme, Turmeric and White pepper were highly potent inhibitors of TPA-induced mouse ear edema. Moreover, antitumor-promoting activity-guided the separation of the relatively active spices led to the isolation of four compds., including ursolic acid from Sage, luteolin from Celery seed, laxogenin from Xiebai and piperine from White pepper. These compds. along with capsaicin were also found to inhibit TPA-induced mouse ear edema.

IT 491-70-3P, Luteolin  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (of Celery seed; cancer chemoprevention by spice constituents as determined by tetradecanoyl-phorbol-13-acetate (TPA)-enhanced 3H-choline incorporation into phospholipids in C3H10T1/2 cells and TPA-induced mouse ear edema)  
 RN 491-70-3 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)

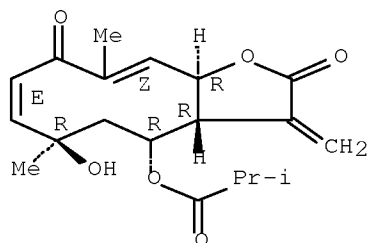


L75 ANSWER 25 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1996:81169 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 124:170558  
 TITLE: An artemisinin acid analog from *Tithonia diversifolia*  
 AUTHOR(S): Bordoloi, Manobjyoti; Barua, Nabin C.; Ghosh, Anil C.  
 CORPORATE SOURCE: Natural Products Chem. Group, Regional Res. Lab., Assam, 785006, India  
 SOURCE: Phytochemistry (1996), 41(2), 557-9  
 CODEN: PYTCAS; ISSN: 0031-9422  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB A new artemisinin acid analog compound has been isolated from mature stems of *Tithonia diversifolia* and its structure determined as (I).  
 IT 59979-56-5, Tagitinin C  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)  
 (from *Tithonia diversifolia*)  
 RN 59979-56-5 CAPLUS  
 CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as described by E or Z.



L75 ANSWER 26 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1994:431140 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 121:31140  
 TITLE: Germination and growth inhibitory sesquiterpene  
 lactones and a flavone from *Tithonia diversifolia*  
 AUTHOR(S): Baruah, Narayan C.; Sarma, Jadab C.; Barua, Nabin C.;  
 Sarma, Soneswar; Sharma, Ram P.  
 CORPORATE SOURCE: Nat. Prod. Chem. Div., Reg. Res. Lab., Jorhat, 785  
 006, India  
 SOURCE: Phytochemistry (1994), 36(1), 29-36  
 CODEN: PYTCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

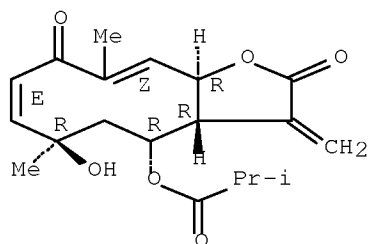
AB Inhibitory effects of two sesquiterpene lactones, tagitinin A, tagitinin C,  
 and a flavonoid, hispidulin, isolated from *T. diversifolia* were determined on  
 germination of radish, cucumber and onion seeds. The flavonoid hispidulin was  
 more toxic to the crop seeds tested and the activity of tagitinin C was weaker  
 than that of tagitinin A and hispidulin. Seventeen derivs. have been prepared  
 from tagitinin A and C by chemical transformation and their phytotoxicity has  
 been compared with the parent compds. (all at 250  $\mu$ M) using radish seeds. The  
 structural requirements related to their biol. activity have also been  
 delineated.

IT 59979-56-5, Tagitinin C  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); BIOL (Biological study)  
 (from *Tithonia diversifolia*, germination and growth inhibitory activity  
 of)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-  
 octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-  
 yl ester (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as described by E or Z.



L75 ANSWER 27 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:106074 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 120:106074

TITLE: Magnesium iodide-diethyl ether-acetic anhydride: a new and efficient acylating system for primary, secondary and tertiary alcohols and phenols

AUTHOR(S): Chowdhury, Pritish K.

CORPORATE SOURCE: Natl. Prod. Chem. Div., Reg. Res. Lab., Jorhat, 785 006, India

SOURCE: Journal of Chemical Research, Synopses (1993), (8), 338-9

CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:106074

AB Primary, secondary and tertiary alcs. are rapidly acetylated by a magnesium iodide-acetic anhydride system at room temperature while phenols are likewise acetylated in quant. yields but under reflux in di-Et ether.

IT 59979-56-5

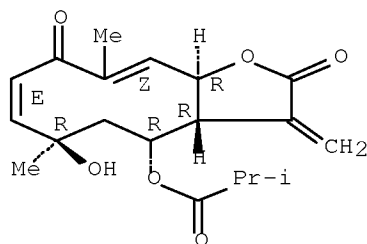
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acetylation of, with magnesium iodide-acetic anhydride system)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 28 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:556217 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 119:156217

TITLE: Insect feeding deterrents from *Tithonia diversifolia* (Hemsl) Gray

AUTHOR(S): Dutta, P.; Chaudhuri, R. P.; Sharma, R. P.

CORPORATE SOURCE: Reg. Res. Lab., (CSIR), Jorhat, India

SOURCE: Journal of Environmental Biology (1993), 14(1), 27-33

CODEN: JEBIDP; ISSN: 0254-8704

DOCUMENT TYPE: Journal

LANGUAGE: English

AB *Tithonia diversifolia*, commonly known as Mexican sunflower, of the family Asteraceae (Compositae) is a feeding deterrent of insect pests. The major compds. - tagitinin A, tagitinin C and hispidulin - isolated from the plant

exhibited dose dependent feeding deterrence when evaluated against caterpillars of *Diacrisia obliqua* (Lepidoptera: Arctiidae); *Phissama transiens* (Lepidoptera: Arctiidae); *Trabala vishnu* (Lepidoptera: Lasiocampidae) and grubs of *Epilachna vigintioctopunctata* (Coleoptera: Coccinellidae).

IT 59979-56-5, Tagitinin C

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

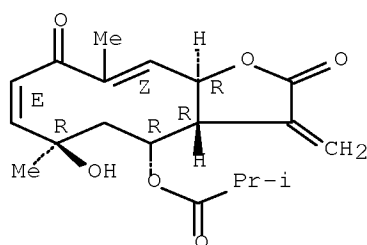
(of *Tithonia diversifolia*, insect feeding inhibiting activity of)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 29 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:165170 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 118:165170

TITLE: Chemotaxonomic analysis of *Pappobolus* (Asteraceae: Heliantheae)

AUTHOR(S): Spring, Otmar; Panero, Jose L.; Schilling, Edward E.

CORPORATE SOURCE: Inst. Biol. I, Univ. Tuebingen, Tuebingen, D-7400, Germany

SOURCE: Biochemical Systematics and Ecology (1992), 20(7), 671-84

CODEN: BSECBU; ISSN: 0305-1978

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chemical constituents from capitate glandular trichomes were analyzed for 33 of the 38 species of *Pappobolus*. In total, 35 HPLC peaks were detected, 30 of which could be tentatively assigned to known compds. of the sesquiterpene lactone and benzofuran type. Compds. of the 1-keto-2,3-unsatd.-furanoheliangolide type (budleins) were present in all plants and quant. dominated the compound patterns. Several other heliangolides were also present. Xanthanolides were detected in about 50% of the species, and benzofurans from about two-thirds of them. *Pappobolus* is the only genus for which benzofurans have been demonstrated to occur in capitate glandular trichomes. Overall there was a high degree of chemical homogeneity, which is in accord with the suggestion that *Pappobolus* is monophyletic and of relatively recent origin. *Pappobolus* is distinct from other genera of the subtribe Helianthinae in the occurrence of xanthanolides and in the lack of germacrolides and eudesmanolides.

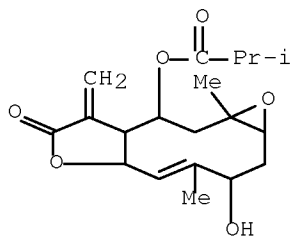
IT 59979-58-7, Tagitinin E

RL: BIOL (Biological study)

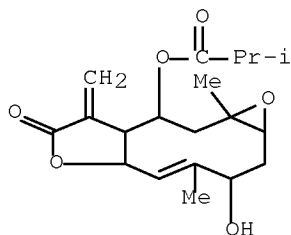
(of *Pappobolus* glandular trichomes, taxonomy in relation to)

RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-  
1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-  
oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 30 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1992:648547 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 117:248547  
 TITLE: Sesquiterpene lactones from two Tithonia species  
 AUTHOR(S): Schuster, A.; Stokes, S.; Papastergiou, F.; Castro, V.; Poveda, L.; Jakupovic, J.  
 CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D-1000/12, Germany  
 SOURCE: Phytochemistry (1992), 31(9), 3139-41  
 CODEN: PYTCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB From two Tithonia species, in addition to known compds., nine new sesquiterpene lactones were isolated: eight germacranolides and one eudesmanolide. The structures were elucidated by means of spectroscopic methods.  
 IT 144302-13-6  
 RL: PROC (Process)  
 (structure and isolation of, from Tithonia diversifolia)  
 RN 144302-13-6 CAPLUS  
 CN Propanoic acid, 2-methyl-, 1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester, [1aR-(1aR\*,3R\*,4Z,5aR\*,8aR\*,9R\*,10aR\*)]- (9CI) (CA INDEX NAME)



L75 ANSWER 31 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1991:603272 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 115:203272  
 TITLE: A phytochemical investigation of medicinal plants of the Compositae from Rwanda

AUTHOR(S): Mungarulire, J.  
 CORPORATE SOURCE: IRST/CURPHAMETRA, Butare, Rwanda  
 SOURCE: Herba Hungarica (1990), 29(3), 73-8  
 CODEN: HEHUAW; ISSN: 0018-0580  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB In the course of an investigation of the widespread Compositae family, five medicinal plants from Rwanda were studied. Those plants were particularly screened for an showed moderate antimicrobial and significant cytotoxic activities. Most of the active principles were found to be highly oxygenated sesquiterpene lactones, e.g., tagitinin C and F. In one case, a polyhydroxylated sapogenin was responsible for the cytotoxic activity. Some flavonoids were also isolated along with the sesquiterpene lactones.

IT 59979-57-6 59979-58-7

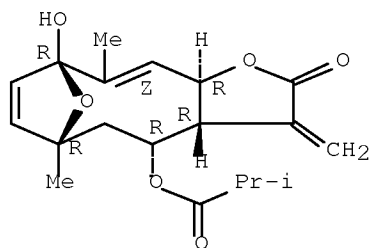
RL: BIOL (Biological study)  
 (of *Tithonia diversifolia*, isolation, and neoplasm inhibiting activity of)

RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

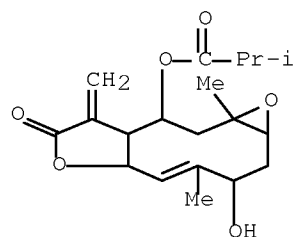
Absolute stereochemistry.

Double bond geometry as described by E or Z.



RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 32 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:510605 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 115:110605

TITLE: Sesquiterpene lactones and benzofurans in glandular trichomes of three Pappobolus species

AUTHOR(S): Spring, Otmar; Vargas, David; Fischer, Nikolaus H.  
 CORPORATE SOURCE: Inst. Biol. I, Univ. Tuebingen, Tuebingen, D-7400, Germany  
 SOURCE: Phytochemistry (1991), 30(6), 1861-7  
 CODEN: PYTCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

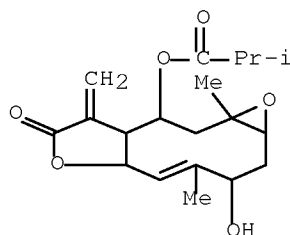
AB Twenty-four sesquiterpene lactones and 4 benzofurans were isolated and identified in glandular trichomes of 3 Pappobolus species. Among them several new furanoheliangolides and xanthanolides were found. The localization of benzofurans together with the sesquiterpene lactones in special glandular hairs of the leaf surface and parts of the inflorescence was demonstrated. A recently developed microsampling technique allowed for a rapid survey and selection of the plant material in order to obtain information on the whole genus for a chemotaxonomic investigation.

IT 59979-58-7

RL: BIOL (Biological study)  
 (of *Viguiera acutifolia* and *Helianthopsis sagasteguii*)

RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-  
 1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 33 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:203526 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 114:203526

TITLE: Sesquiterpene lactones from *Helianthus tuberosus*

AUTHOR(S): Spring, Otmar

CORPORATE SOURCE: Inst. Biol., Univ. Tuebingen, Tuebingen, 7400, Germany

SOURCE: Phytochemistry (1991), 30(2), 519-22

CODEN: PYTCAS; ISSN: 0031-9422

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A chemical anal. of the resinous content of capitate glandular trichomes from the leaf surface of *H. tuberosus* established the existence of 19 sesquiterpene lactones. Despite a high degree of intraspecific variation, comparison of the compound patterns of 12 different specimens by means of a microsampling technique and successive HPLC anal. indicated the occurrence of two chemotypes with distinct sesquiterpene lactone profiles. While plants of the one type are characterized by the dominance of 1,10-epoxidized heliangolides, the second group is composed of specimens which particularly accumulate 1-keto-2,3-unsatd.-furanoheliangolides. Biosynthetic and chemotaxonomic aspects are briefly discussed.

IT 59979-58-7, Tagitinin E

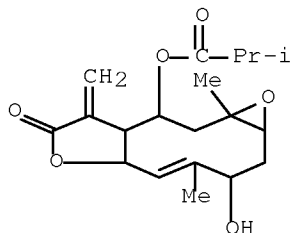
RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

BIOL (Biological study); OCCU (Occurrence)

(of *Helianthus tuberosus*)

RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-  
1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-  
oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 34 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:129083 CAPLUS Full-text

DOCUMENT NUMBER: 114:129083

TITLE: Anticancer agents containing tagitinin C

INVENTOR(S): Ikegawa, Tetsuo; Ikegawa, Nobuo; Okuma, Akihiro

PATENT ASSIGNEE(S): Tsumura and Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

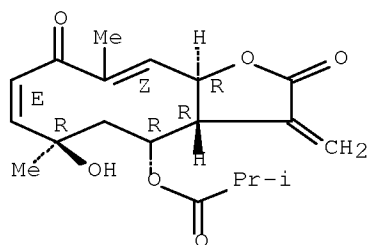
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02264722	A	19901029	JP 1989-83907	19890404 <--
PRIORITY APPLN. INFO.:			JP 1989-83907	19890404 <--
AB Anticancer agents contain tagitinin C (I) as an active ingredient. I (extracted from <i>Tithonia diversifolia</i> ) showed IC50 of 0.52, 0.17, and 0.24 µg/mL against Hela-S3, L-5178Y, and L-1210, resp. LD50 of I was >2 g/kg p.o. and 150 mg/kg i.p. in mice. Tablets were formulated containing corn starch 44, crystalline cellulose 40, CMC Ca 5, silica 0.5, Mg stearate 0.5, and I 10 g.				
IT 59979-56-5, Tagitinin C				
RL: BIOL (Biological study)				
(as anticancer agent)				
RN 59979-56-5 CAPLUS				
CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)				

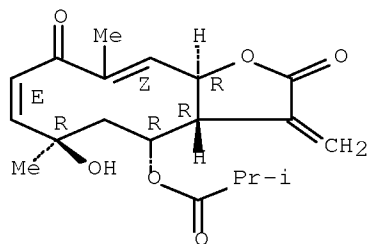
Absolute stereochemistry.

Double bond geometry as described by E or Z.



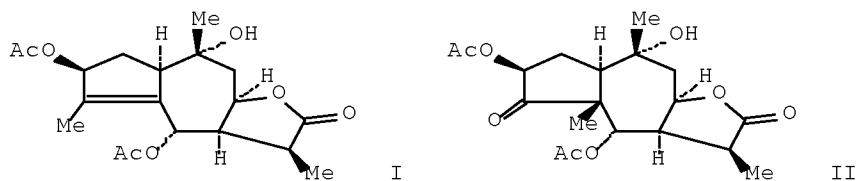
L75 ANSWER 35 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1991:6942 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 114:6942  
 TITLE: Magnesium-iodine-diethyl ether: an efficient system  
 for the deoxygenation of oxiranes to olefins  
 AUTHOR(S): Chowdhury, Pritish K.  
 CORPORATE SOURCE: Nat. Prod. Chem. Div., Reg. Res. Lab., Jorhat, 785  
 006, India  
 SOURCE: Journal of Chemical Research, Synopses (1990  
 ), (6), 192-3  
 CODEN: JRPSDC; ISSN: 0308-2342  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 114:6942  
 AB The system Mg-iodine-Et<sub>2</sub>O deoxygenates oxiranes into the corresponding olefins  
 in excellent yield and with retention of configuration.  
 IT 59979-56-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, from epoxide)  
 RN 59979-56-5 CAPLUS  
 CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-  
 octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-  
 yl ester (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as described by E or Z.



L75 ANSWER 36 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1989:574424 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 111:174424  
 TITLE: Biomimetic transformation of a guaianolide to a  
 pseudoguaianolide  
 AUTHOR(S): Bordoloi, Manobjyoti; Sarmah, Jadab C.; Sharma, Ram P.  
 CORPORATE SOURCE: Nat. Prod. Chem. Div., Reg. Res. Lab., Assam, India  
 SOURCE: Tetrahedron (1989), 45(1), 289-302

DOCUMENT TYPE: JOURNAL  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 111:174424  
 GI



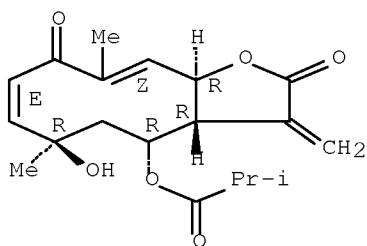
AB The long-awaited transformation of the guaianolide skeleton, e.g., I, to the pseudoguaianolide skeleton, e.g., II, was achieved. During this study two new carbon skeletons in sesquiterpene lactones were also prepared

IT 59979-56-5  
 RL: PROC (Process)  
 (conversion of, to pseudoguaianolide via guaianolide)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as described by E or Z.



L75 ANSWER 37 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:62551 CAPLUS Full-text

DOCUMENT NUMBER: 108:62551

TITLE: Separations of flavonoids and alkaloids in medicinal herbs by high-speed counter-current chromatography

AUTHOR(S): Zhang, Tianyou; Cai, Dingguo; Ito, Yoichiro

CORPORATE SOURCE: Lab. Tech. Dev., Natl. Heart, Lung, Blood Inst., Bethesda, MD, 20892, USA

SOURCE: Journal of Chromatography (1988), 435(1), 159-66  
 CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Counter-current chromatog. is a new liquid-liquid partition chromatog. without using solid support. The capability of this high-speed counter-current

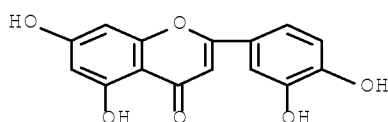
chromatog. was demonstrated on separation of 2 sets of samples obtained from medicinal herbs: a synthetic mixture of 3'-hydroxygenkwanin, luteolin and apigenin was separated on a 2-phase solvent system composed of CHCl<sub>3</sub>-MeOH-H<sub>2</sub>O(4:3:2) and a crude EtOH extract from *Anisodus tangulicus* [CHCl<sub>3</sub>-pH 6.4 0.07M Na phosphate (1:1)]. In the light of chromatograms obtained from these samples, advantages of high-speed counter-current chromatog. over other chromatog. methods were discussed in terms of partition efficiency, peak resolution, separation time, sample loading capacity, etc.

IT 491-70-3F, Luteolin

RL: PUR (Purification or recovery); PREP (Preparation)  
(separation of, in medicinal herbs by high-speed counter-current chromatog.)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



L75 ANSWER 38 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:551218 CAPLUS Full-text

DOCUMENT NUMBER: 107:151218

TITLE: Germacranolides, guaianolides and eudesmanolides from *Greenmaniella resinosa*

AUTHOR(S): Zdero, C.; Bohlmann, F.; Scott, R.

CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D-1000/12, Fed. Rep. Ger.

SOURCE: Phytochemistry (1987), 26(7), 1999-2006

CODEN: PYTCAS; ISSN: 0031-9422

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The aerial parts of *G. resinosa* afforded, in addition to known compds., 22 new ones: 9 germacranolides, 7 eudesmanolides, 5 guaianolides, and a bisabolene derivative. The structures were elucidated by spectroscopic methods and by some chemical transformations including partial synthesis. The chemotaxonomic situation of *Greenmaniella* and the biogenetic relationships of the compds. are discussed briefly.

IT 59979-56-5, Tagitinin C 59979-57-6, Tagitinin F  
59979-58-7, Tagitinin E

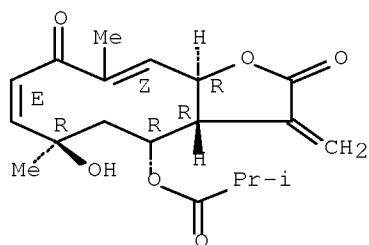
RL: BIOL (Biological study)  
(from *Greenmaniella resinosa*)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.

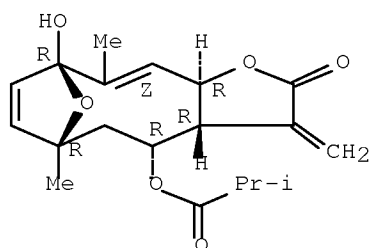


RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

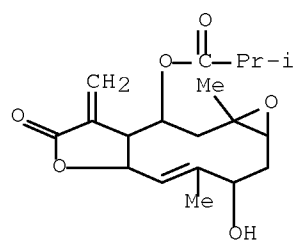
Absolute stereochemistry.

Double bond geometry as described by E or Z.



RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



IT 110382-29-1 110382-30-4

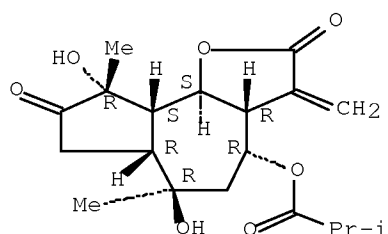
RL: BIOL (Biological study)

(from Greenmaniella resinosa, isolation and structure determination of)

RN 110382-29-1 CAPLUS

CN Propanoic acid, 2-methyl-, dodecahydro-6,9-dihydroxy-6,9-dimethyl-3-methylene-2,8-dioxoazuleno[4,5-b]furan-4-yl ester, [3aR-(3aα,4β,6α,6aα,9β,9aα,9bβ)]- (9CI)  
(CA INDEX NAME)

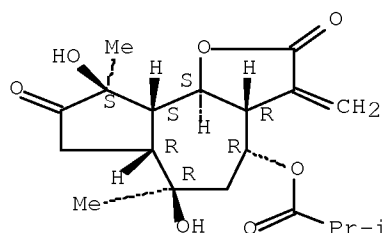
Absolute stereochemistry.



RN 110382-30-4 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,6aR,9S,9aS,9bS)-dodecahydro-6,9-dihydroxy-6,9-dimethyl-3-methylene-2,8-dioxoazuleno[4,5-b]furan-4-yl ester  
(CA INDEX NAME)

Absolute stereochemistry.



IT 110390-87-9P

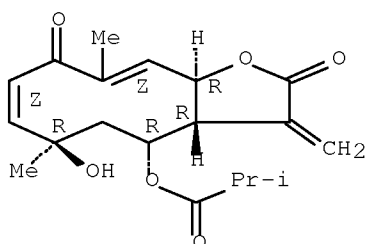
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and transformation of)

RN 110390-87-9 CAPLUS

CN Propanoic acid, 2-methyl-, 2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester,  
[3aR-(3aR\*,4R\*,6R\*,7Z,10Z,11aR\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



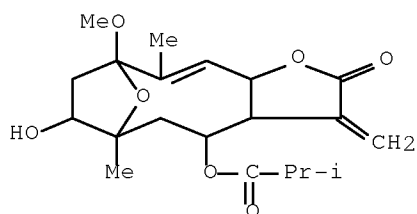
IT 110382-31-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

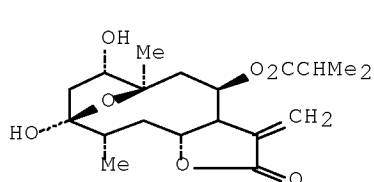
RN 110382-31-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7R,9R,10Z,11aR)-2,3,3a,4,5,6,7,8,9,11a-decahydro-7-hydroxy-9-methoxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (9CI) (CA INDEX NAME)

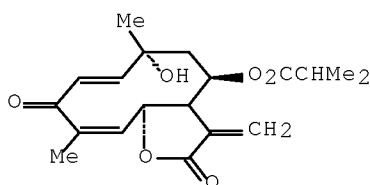
NAME)



L75 ANSWER 39 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1986:420472 CAPLUS Full-text  
 DOCUMENT NUMBER: 105:20472  
 ORIGINAL REFERENCE NO.: 105:3369a,3372a  
 TITLE: Feeding deterrents for *Philosamia ricini* (*Samia cynthia* subsp. *ricini*) from *Tithonia diversifolia*  
 AUTHOR(S): Dutta, P.; Bhattacharyya, P. R.; Rabha, L. C.; Bordoloi, D. N.; Barua, N. C.; Chowdhury, P. K.; Sharma, R. P.; Barua, J. N.  
 CORPORATE SOURCE: Div. Med. Econ. Plants, Reg. Res. Lab., Jorhat, 785006, India  
 SOURCE: *Phytoparasitica* (1986), 14(1), 77-80  
 CODEN: PHPRA2; ISSN: 0334-2123  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

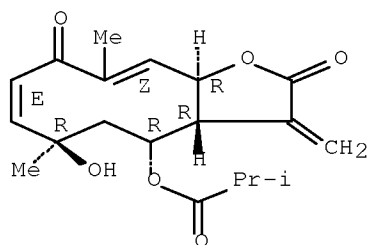


II

AB Tagitinin A (I) [59979-61-2] and C (II) [59979-56-5] and hispidulin [1447-88-7] isolated from *T. diversifolia* were potent feeding deterrents, when evaluated against 4th instar caterpillars of the Eri-silkworm (*P. ricini*) (Lepidoptera: Saturnidae); tagitinin F [59979-57-6] was not.  
 IT 59979-56-5  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
 (feeding inhibiting activity of, for *Philosamia ricini*)  
 RN 59979-56-5 CAPLUS  
 CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



IT 59979-57-6

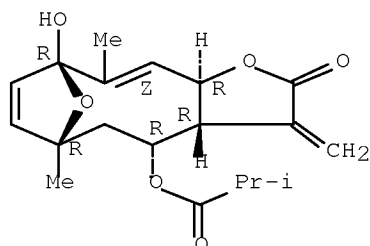
RL: BOC (Biological occurrence); BSU (Biological study, unclassified);  
BIOL (Biological study); OCCU (Occurrence)  
(of *Tithonia diversifolia*)

RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 40 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:471530 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 103:71530

ORIGINAL REFERENCE NO.: 103:11520h,11521a

TITLE: Structure-activity relationship: synthesis of  
10-deoxytagitinin C and 10-deoxycyclotagitinin C and  
their anti-feedant properties

AUTHOR(S): Sarma, Debendra N.; Barua, Nabin C.; Sharma, Ram P.

CORPORATE SOURCE: Reg. Res. Lab., CSIR, Assam, India

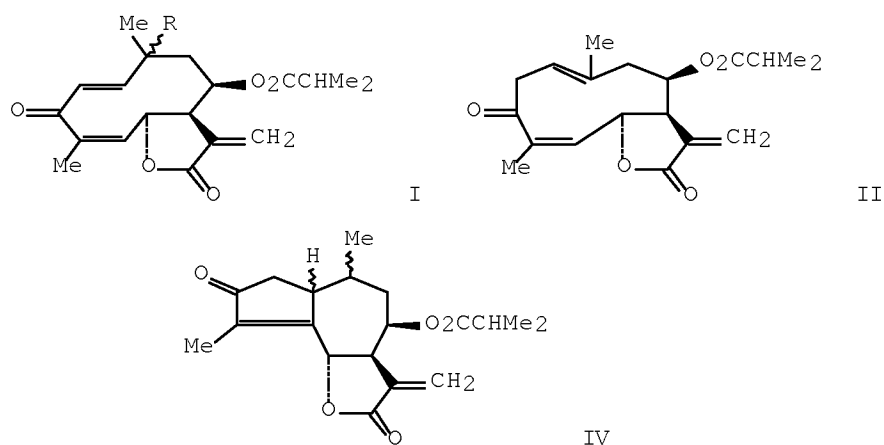
SOURCE: Chemistry & Industry (London, United Kingdom) (  
1985), (5), 167-8

CODEN: CHINAG; ISSN: 0009-3068

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Reaction of tagitinin C (I, R =  $\alpha$ -OH) with Zn/HOAc gave the diene lactone II, which in MeCN was treated with Me<sub>3</sub>SiCl and NaI to give 10-deoxytagitinin C (I, R = H) (III), which cyclized in boiling MeCN containing SnCl<sub>4</sub> to give 10-deoxycyclotagitinin C (IV). III and IV were 10 times less active as antifeedants against *Philasomia ricini* than tagitinin C and cyclotagitinin C.

IT 59979-56-5

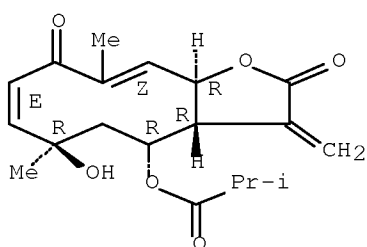
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 41 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:182384 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 102:182384

ORIGINAL REFERENCE NO.: 102:28567a,28570a

TITLE: Sesquiterpene lactones from the *Calea* genus:

caleinolides, a special type of heliangolides

AUTHOR(S): Borges del Castillo, J.; Manresa Ferrero, M. T.;  
Rodriguez Luis, F.; Rodriguez Ubis, J. C.; Vazquez  
Bueno, P.

CORPORATE SOURCE: Fac. Cienc., Univ. Auton. Madrid, Madrid, Spain

SOURCE: Revista Latinoamericana de Quimica (1984),  
15(3-4), 96-106

CODEN: RLAQA8; ISSN: 0370-5943

DOCUMENT TYPE: Journal

LANGUAGE: Spanish

AB The name caleinolides is suggested for a class of heliangolides from *Calea* and *Neurolana* species. The finding is based on NMR spectra of 58 compds. and on chemical conversions. Neurolenin A and B (Vazquez Bueno, P., et al., 1982) were the reference compds. The structures are characteristic for trans-heliangolides. The OH or ester groups at C-8 and C-9 are trans, with orientations  $8\beta$  and  $9\alpha$ .

IT 59979-56-5

RL: BIOL (Biological study)

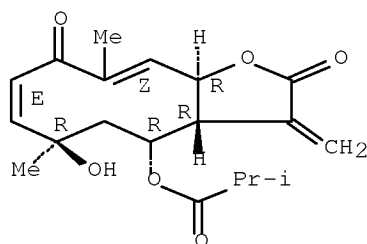
(of *Calea*, NMR spectrum of)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 42 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:24388 CAPLUS Full-text

DOCUMENT NUMBER: 102:24388

ORIGINAL REFERENCE NO.: 102:4015a,4018a

TITLE: Reductive removal of the tert-hydroxy group in  $\alpha,\beta$ -unsaturated  $\gamma$ -tert-hydroxyketones

with chlorotrimethylsilane-sodium iodide. An alternative to zinc-acetic acid reduction

AUTHOR(S): Sarma, Debendra N.; Sarma, Jadab C.; Barua, Nabin C.; Sharma, Ram P.

CORPORATE SOURCE: Div. Nat. Prod.Chem., Reg. Res. Lab., Jorhat, 785 006, India

SOURCE: Journal of the Chemical Society, Chemical Communications (1984), (13), 813-14

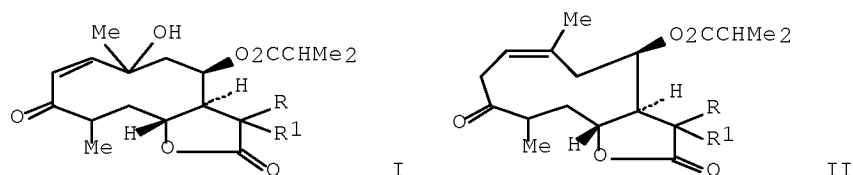
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:24388

GI



AB Me<sub>3</sub>SiCl-NaI effected reductive removal of the tert-OH group from a variety of cyclic title hydroxy ketones. E.g., stirring the hydroxy ketone I (RR<sub>1</sub> = CH<sub>2</sub>) in dry MeCN with a 2:1 mixture of NaI and Me<sub>3</sub>SiCl at room temperature for 10 min gave the ketone II (RR<sub>1</sub> = CH<sub>2</sub>) in 90% yield. Similarly, I (R = Me, MeOCH<sub>2</sub>, R<sub>1</sub> = H) gave 90% II (R, R<sub>1</sub> as before).

IT 59979-56-5

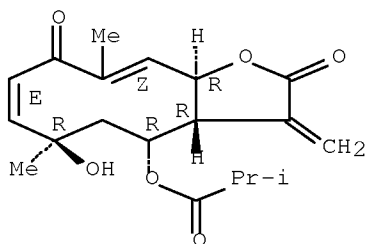
RL: RCT (Reactant); RACT (Reactant or reagent)  
(dehydroxylation of, by chlorotrimethylsilane-sodium iodide)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 43 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:438228 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 101:38228

ORIGINAL REFERENCE NO.: 101:5969a,5972a

TITLE: Cleavage of tert-methylthiomethyl ethers

AUTHOR(S): Sarma, Debendra N.; Barua, Nabin C.; Sharma, Ram P.

CORPORATE SOURCE: Div. Nat. Prod. Chem., Reg. Res. Lab., Assam, India

SOURCE: Chemistry & Industry (London, United Kingdom) (

1984), (6), 223-4

CODEN: CHINAG; ISSN: 0009-3068

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Methylthiomethyl ethers of tertiary OH groups in sensitive natural products were cleaved by treatment with Hg(OAc)<sub>2</sub>-MeCN to give the acetoxymethyl ethers in 75-80% yield. The latter were heated with H<sub>2</sub>O to give .apprx.95% of the free alcs.

IT 59979-56-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(methylthiomethyl ether cleavage in preparation of)

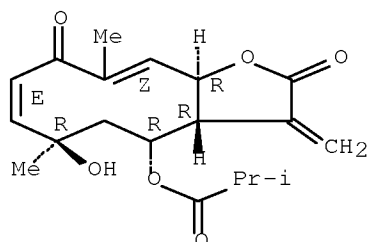
RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-

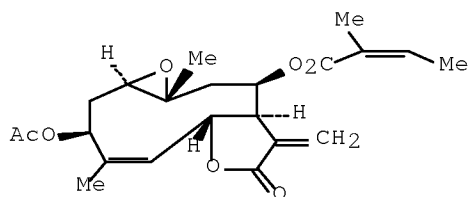
octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

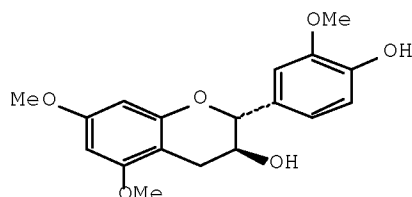
Double bond geometry as described by E or Z.



L75 ANSWER 44 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1984:435877 CAPLUS Full-text  
 DOCUMENT NUMBER: 101:35877  
 ORIGINAL REFERENCE NO.: 101:5573a,5576a  
 TITLE: Terpenoids and a flavan-3-ol from *Viguiera quinquerradiata*  
 AUTHOR(S): Delgado, Guillermo; Alvarez, Laura; Romo de Vivar, Alfonso  
 CORPORATE SOURCE: Inst. Quim., Univ. Nac. Auton. Mexico, Mexico City, 04510, Mex.  
 SOURCE: Phytochemistry (Elsevier) (1984), 23(3), 675-8  
 CODEN: PYTCAS; ISSN: 0031-9422  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I



II

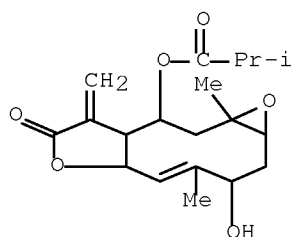
AB The new compds. acetyllepocarpin (I) and the flavan-3-ol II were isolated from *Viguiera quinquerradiata* and their structures were determined by standard chemical and spectral methods. Diterpenes 15 $\alpha$ -angeloyloxy- and 15 $\alpha$ -tigloyloxy-ent-kaur-16-en-19-oic acid and sesquiterpene lactones lepocarpin and budlein A were also found.

IT 59979-58-7

RL: PRP (Properties)  
 (NMR of carbon-13 of)

RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 45 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:206486 CAPLUS Full-text

DOCUMENT NUMBER: 100:206486

ORIGINAL REFERENCE NO.: 100:31309a,31312a

TITLE: Heliangolides and trachylobane and villanovane derivatives from *Viguiera* species

AUTHOR(S): Bohlmann, Ferdinand; Zdero, Christa; Schmeda-Hirschmann, Guillermo; Jakupovic, Jasmin; Castro, Victor; King, Robert M.; Robinson, Harold

CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D-1000/12, Fed. Rep. Ger.

SOURCE: Liebigs Annalen der Chemie (1984), (3), 495-502

CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE: Journal

LANGUAGE: German

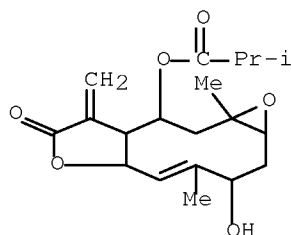
AB From the aerial parts of *V. cordata*, in addition to budlein A and isoatripliciolide, 2 further heliangolides were isolated. The aerial parts of *V. pazensis* afforded in addition to known compds. 3 trachylobane derivs., as well as a further villanovane derivative. The structures were elucidated by spectroscopic methods and some chemical transformations.

IT 59979-58-7

RL: BIOL (Biological study)  
(from *Viguiera*)

RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)

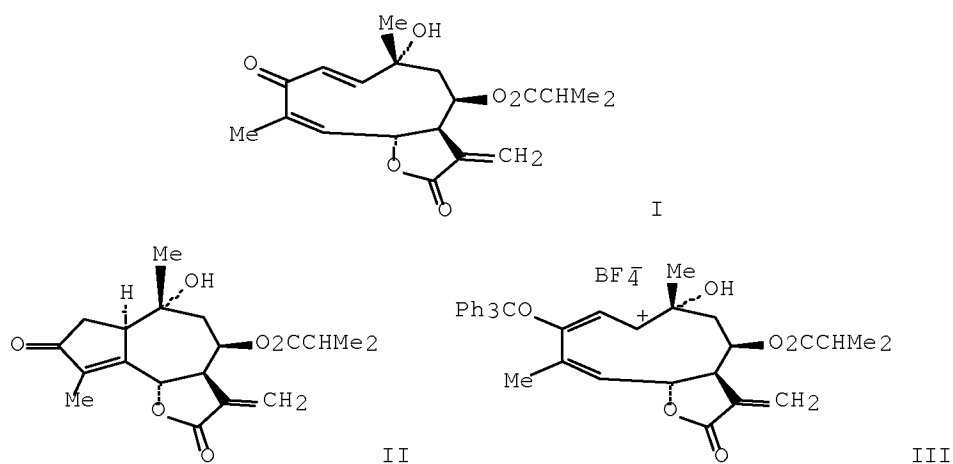


L75 ANSWER 46 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:192088 CAPLUS Full-text

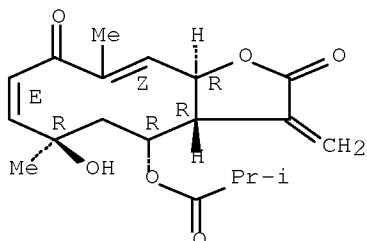
DOCUMENT NUMBER: 100:192088

ORIGINAL REFERENCE NO.: 100:29211a,29214a  
 TITLE: Cyclization of tagitinin C (germacranolide) to cyclotagitinin C (guaianolide) with trityl tetrafluoroborate: a new cyclizing agent  
 AUTHOR(S): Chowdhury, Pritish K.; Sharma, Ram P.; Baruah, Jogendra N.  
 CORPORATE SOURCE: Div. Nat. Prod. Chem., Reg. Res. Lab., Jorhat, 785 006, India  
 SOURCE: Chemistry & Industry (London, United Kingdom) (1983), (24), 927-8  
 CODEN: CHINAG; ISSN: 0009-3068  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 100:192088  
 GI

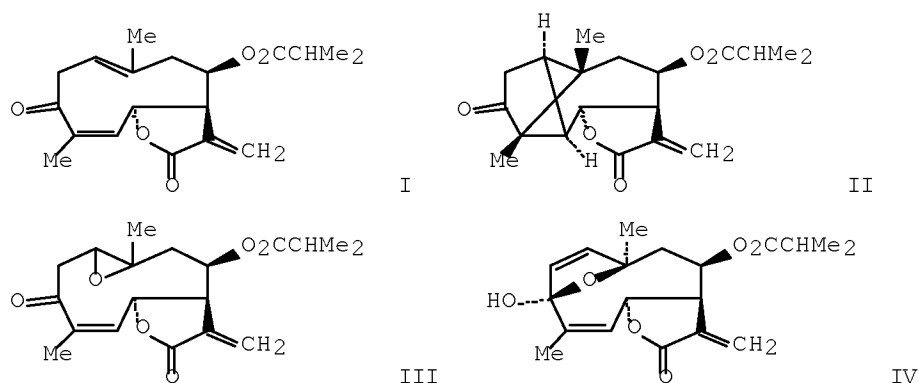


AB Treatment of tagitinin C (I) in  $\text{CH}_2\text{Cl}_2$  with  $\text{Ph}_3\text{C}^+\text{BF}_4^-$  at room temperature for 10 min gave 95% cyclotagitinin C (II), presumably via the enol ether III.  
 IT 59979-56-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of, to cyclotagitinin C)  
 RN 59979-56-5 CAPLUS  
 CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as described by E or Z.



L75 ANSWER 47 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1984:139370 CAPLUS Full-text  
 DOCUMENT NUMBER: 100:139370  
 ORIGINAL REFERENCE NO.: 100:21283a,21286a  
 TITLE: Photocyclization of a heliangolide - a cyclodecadienone  
 AUTHOR(S): Chowdhury, P. K.; Sharma, R. P.; Baruah, J. N.  
 CORPORATE SOURCE: Div. Nat. Prod. Chem., Reg. Res. Lab., Jorhat, 785 006, India  
 SOURCE: Tetrahedron Letters (1983), 24(48), 5429-32  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Irradiation of the heliangolide I with a bare arc Hg lamp through quartz gave the cyclization product II, whereas the corresponding epoxide III gave tagitinin F (IV).

IT 59979-57-6P

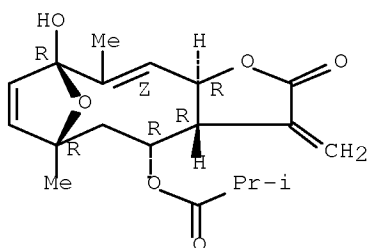
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by photocyclization of epoxyheliangolide)

RN 59979-57-6 CAPLUS

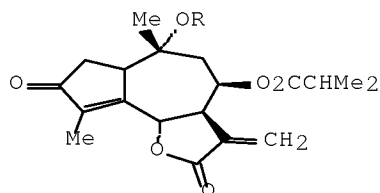
CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

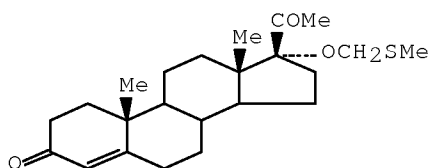
Double bond geometry as described by E or Z.



L75 ANSWER 48 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1984:103657 CAPLUS Full-text  
 DOCUMENT NUMBER: 100:103657  
 ORIGINAL REFERENCE NO.: 100:15761a,15764a  
 TITLE: A new method for deprotection of methylthiomethyl  
 ethers  
 AUTHOR(S): Chowdhury, P. K.; Sharma, R. P.; Baruah, J. N.  
 CORPORATE SOURCE: Div. Nat. Prod. Chem., Reg. Res. Lab., Jorhat, 6,  
 India  
 SOURCE: Tetrahedron Letters (1983), 24(41), 4485-6  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I



II

AB Stirring a solution of sesquiterpene I (R = CH<sub>2</sub>SMe) in CH<sub>2</sub>Cl<sub>2</sub> with trityl tetrafluoroborate for 5 min at room temperature followed by treatment with H<sub>2</sub>O gave 95% the corresponding alc. I (R = H). Seven other methylthiomethyl ethers, e.g., Me(CH<sub>2</sub>)<sub>14</sub>CH<sub>2</sub>OCH<sub>2</sub>SMe, pregnenedione derivative II, Me<sub>2</sub>C:CHCH<sub>2</sub>CH<sub>2</sub>CMe(OCH<sub>2</sub>SMe)CH:CH<sub>2</sub>, were deprotected similarly. However, methylthiomethyl ethers of phenols, e.g., α- and β-naphthols, were not cleaved under the reaction conditions.

IT 59979-56-5P

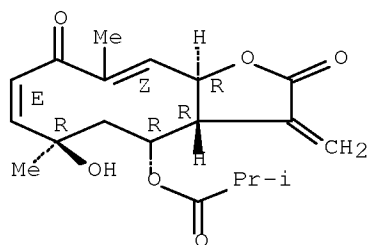
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by deprotection of methylthiomethyl ether)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 49 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1983:522668 CAPLUS Full-text

DOCUMENT NUMBER: 99:122668

ORIGINAL REFERENCE NO.: 99:18901a,18904a

TITLE: Absolute stereochemistry of tagitinin F

AUTHOR(S): Chowdhury, P. K.; Sharma, R. P.; Barua, J. N.

CORPORATE SOURCE: Reg. Res. Lab., CSIR, Jorhat, 785 006, India

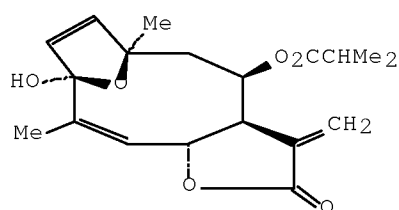
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(4), 402

CODEN: IJSBDB; ISSN: 0376-4699

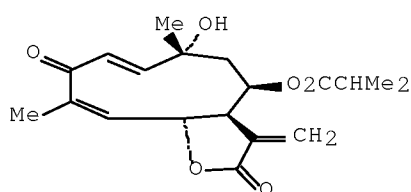
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



II

AB The absolute stereostructure of tagitinin F was determined to be I by synthesis from tagitinin C (II) via irradiation of an EtOH or AcOH solution with a 125W Hg lamp for 2 h.

IT 59979-57-6

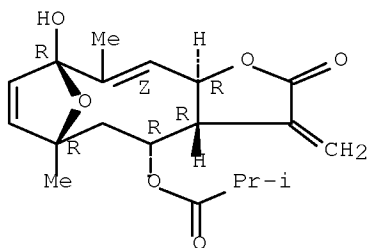
RL: RCT (Reactant); RACT (Reactant or reagent)  
(absolute stereochem. of)

RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



IT 59979-56-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(photochem. isomerization of, to tagitinin F)

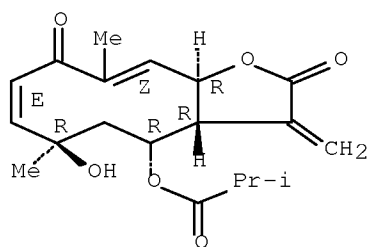
RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-

yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 50 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1983:143670 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 98:143670

ORIGINAL REFERENCE NO.: 98:21901a,21904a

TITLE: Cyclotagitinin C and its transformations

AUTHOR(S): Chowdhury, Pritish K.; Barua, Nabin C.; Sharma, Ram P.; Barua, Jogendra N.; Herz, Werner; Watanabe, Kinzo; Blount, John F.

CORPORATE SOURCE: Reg. Res. Lab., Assam, 785 005, India

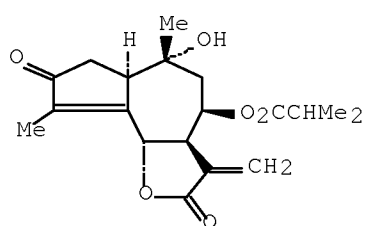
SOURCE: Journal of Organic Chemistry (1983), 48(5), 732-8

CODEN: JOCEAH; ISSN: 0022-3263

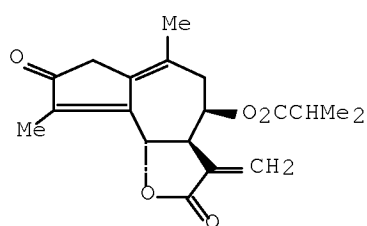
DOCUMENT TYPE: Journal

LANGUAGE: English

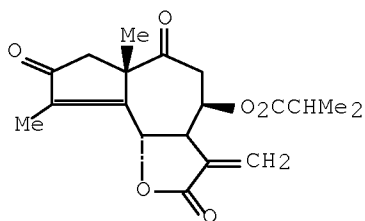
GI



I



II



III

AB The stereochem. previously assigned (Chowdhury, P. K., et al., 1980) to cyclotagitinin C (I) was confirmed. Epoxidn. of anhydrocyclotagitinin C (II) gave two epoxides; the  $\alpha$ -epoxide with Lewis acids resulted in epoxide ring opening with retention of configuration and in rearrangement to a diketone III, whose structure was confirmed by x-ray crystallog. Analogous reactions of

the  $\beta$ -epoxide resulted in epoxide ring opening with inversion of configuration.

IT 59979-56-5

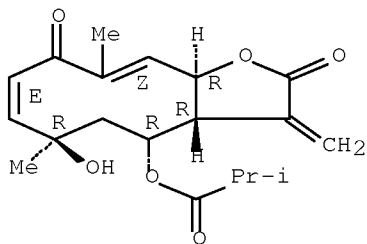
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 51 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:65698 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 96:65698

ORIGINAL REFERENCE NO.: 96:10763a,10766a

TITLE: Isolation of deacetylaviguiestenin and erioflorin from *Helianthus tuberosus*

AUTHOR(S): Morimoto, H.; Oshio, H.

CORPORATE SOURCE: Grad. Sch. Food Med. Sci., Kobe-Gakuin Univ., Kobe, 673, Japan

SOURCE: Journal of Natural Products (1981), 44(6), 748-9

CODEN: JNPRDF; ISSN: 0163-3864

DOCUMENT TYPE: Journal

LANGUAGE: English

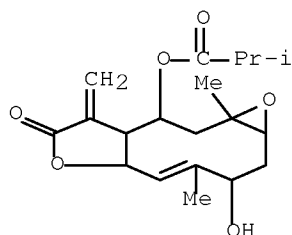
AB Dry leaves of *H. tuberosus* extracted with MeOH yielded heliangin, a known plant growth regulator, deacetylaviguiestenin (tagitinin E), and erioflorin.

IT 59979-58-7

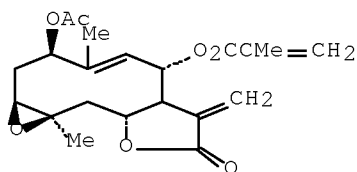
RL: BIOL (Biological study)  
(from Jerusalem artichoke)

RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 52 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1981:202459 CAPLUS Full-text  
 DOCUMENT NUMBER: 94:202459  
 ORIGINAL REFERENCE NO.: 94:32999a,33002a  
 TITLE: Cytotoxicity of some sesquiterpene lactones in vitro  
 AUTHOR(S): Tellez-Martinez, Judith; Taboada, Javier;  
 Gonzalez-Diddi, Manuel  
 CORPORATE SOURCE: Div. Patol., Cent. Med. Nac., Mexico City, Mex.  
 SOURCE: Archivos de Investigacion Medica (1980),  
 11(4), 435-43  
 CODEN: AIVMBU; ISSN: 0066-6769  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English/Spanish  
 GI



I

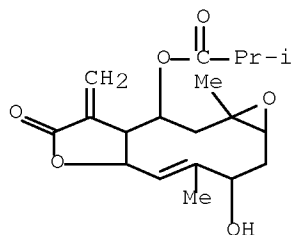
AB Incubation of cell cultures of fibroblasts from mice areolar tissue (L-929) or epithelial cells from human larynx carcinoma (HEp-2) with any of 10 sesquiterpenic lactones (0.1-100 µg/mL) resulted in cytotoxicity as evidenced by inhibition of cell growth. The ED50s for viguiestenin (I) [54153-71-8], zexbrevin A [28644-87-3], zexbrevin B [34302-19-7], budlein A [59481-48-0], calaxin [30412-86-3], and orizabin [34367-14-1] were 5.5, 1, 1, 1, 1, and 4.2 µg/mL, resp. These compds. have potential as anticancer agents. The ED50s of the other 4 lactones tested were 15-66 µg/mL. The mol. structure-activity relationships for each of the lactones are discussed.

IT 59979-58-7

RL: PRP (Properties)  
 (toxicity of, to cultured cells)

RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-  
 1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 53 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:47519 CAPLUS Full-text

DOCUMENT NUMBER: 94:47519

ORIGINAL REFERENCE NO.: 94:7761a,7764a

TITLE: Stereochemistry of ciliarin, zexbrevin, and their relatives

AUTHOR(S): Chowdhury, Pratish K.; Sharma, Ram P.; Thyagarajan, Gopalakrishna; Herz, Werner; Govindan, Serengolam V.

CORPORATE SOURCE: Reg. Res. Lab., Jorhat, 785 006, India

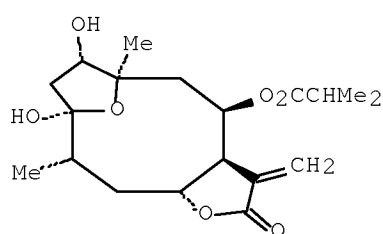
SOURCE: Journal of Organic Chemistry (1980), 45(24), 4993-7

CODEN: JOCEAH; ISSN: 0022-3263

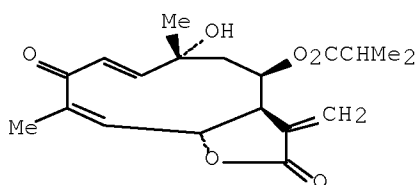
DOCUMENT TYPE: Journal

LANGUAGE: English

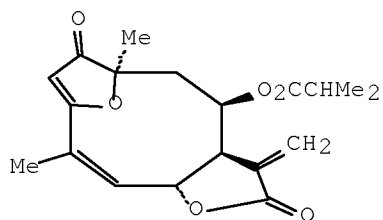
GI



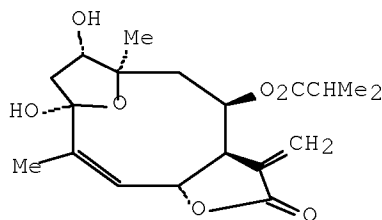
I



II



III



IV

AB Successful interconversions of the sesquiterpene lactones tagitinin A (I), tagitinin C (II), ciliarin (III), and orizabin (IV) are reported and prove that the C-8 stereochem. of ciliarin, orizabin, zexbrevin, zexbrevin B and calaxin is that of the tagitinins, i.e. H-8  $\alpha$ .

IT 59979-56-5

RL: RCT (Reactant); RACT (Reactant or reagent)

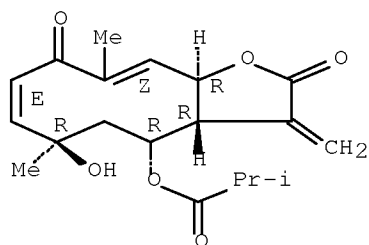
(interconversion between tagitinin A, ciliarin, orizabin, and)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 54 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:76706 CAPLUS Full-text

DOCUMENT NUMBER: 92:76706

ORIGINAL REFERENCE NO.: 92:12647a,12650a

TITLE: Structure of deacetylviguiestenin (tagitinin E). An addendum

AUTHOR(S): Chowdury, Pratish K.; Barua, Nabin C.; Sharma, Ram P.; Thyagarajan, Gopalakrishna; Herz, Werner

CORPORATE SOURCE: Reg. Res. Lab., Jorhat, 78006, India

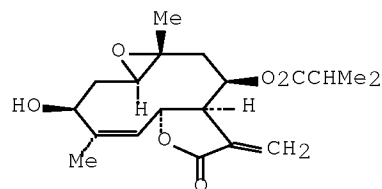
SOURCE: Journal of Organic Chemistry (1980), 45(3), 535-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB The stereochem. assigned to the heliangolide tagitinin E (I) from *Tithonia diversifolia* which is identical with deacetylviguiestenin isolated earlier from *Viguiera stenoloba* was confirmed by correlation with tagitinin C.

IT 59979-56-5

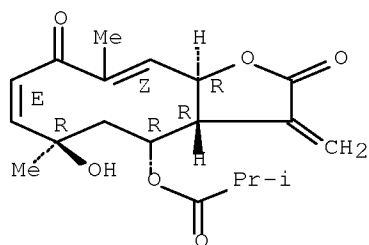
RL: RCT (Reactant); RACT (Reactant or reagent)  
(correlation of deacetylviguiestenin structure with)

RN 59979-56-5 CAPLUS

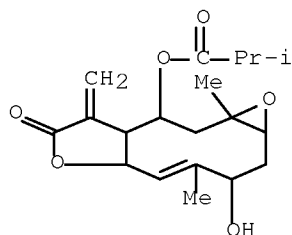
CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

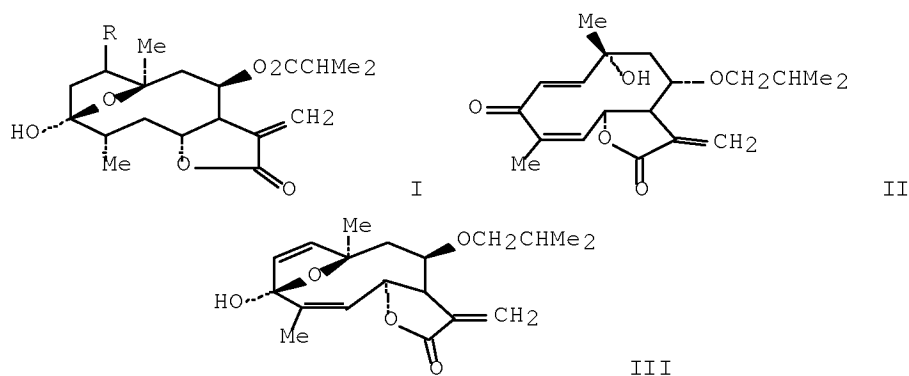
Double bond geometry as described by E or Z.



IT 59979-58-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (stereochem. of, from *Tithonia diversifolia*)  
 RN 59979-58-7 CAPLUS  
 CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-  
 1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-  
 oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 55 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1979:420751 CAPLUS Full-text  
 DOCUMENT NUMBER: 91:20751  
 ORIGINAL REFERENCE NO.: 91:3477a,3480a  
 TITLE: Sesquiterpene lactones of *Tithonia diversifolia*.  
 Stereochemistry of the tagitinins and related  
 compounds  
 AUTHOR(S): Baruah, Nabin C.; Sharma, Ram P.; Madhusudanan, K. P.;  
 Thyagarajan, Gopalakrishna; Herz, Werner; Murari,  
 Ramaswamy  
 CORPORATE SOURCE: Dep. Org. Chem., Reg. Res. Lab., Jorhat, India  
 SOURCE: Journal of Organic Chemistry (1979), 44(11),  
 1831-5  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

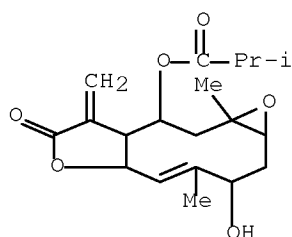


AB Tagitinin A (I, R =  $\alpha$ -OH), C (II), F (III), and tirotundin (I, R = H) were isolated from *T. diversifolia* and their stereochem. and structures confirmed. Addnl. configurations were obtained for tagitinin B and E, zexbrevin, zexbrevin B, orizabin, ciliarin, calaxin, tifruticin, deoxytifruticin, viguiestin, and deacetylviguiestin.

IT 69483-10-9F  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 69483-10-9 CAPLUS

CN Propanoic acid, 2-methyl-, 1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester, [1aR-(1aR\*,3S\*,4Z,5aR\*,8aR\*,9S\*,10aR\*)]- (9CI) (CA INDEX NAME)

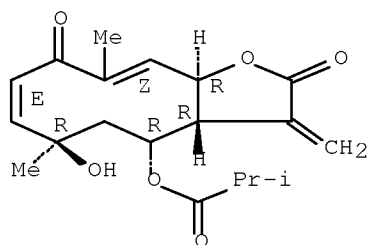


IT 59979-56-5 59979-57-6 59979-58-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(structure and stereochem. of)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as described by E or Z.

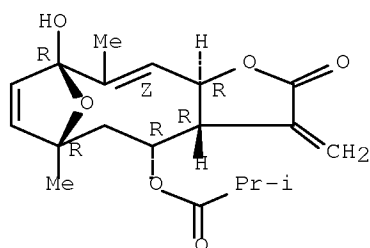


RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

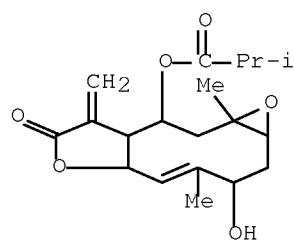
Absolute stereochemistry.

Double bond geometry as described by E or Z.



RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 56 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:152382 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 90:152382

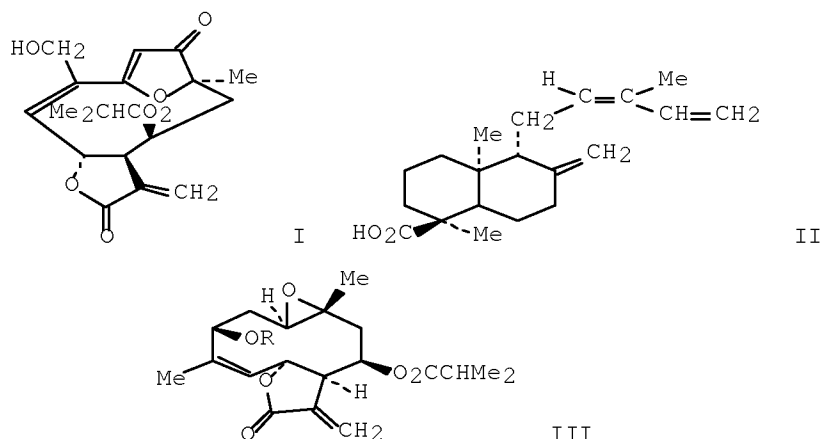
ORIGINAL REFERENCE NO.: 90:24237a,24240a

TITLE: Study of Viguierras. Structure of viguiépinin and correction of viguiéstenin

AUTHOR(S): Romo de Vivar A.; Delgado, G.; Guerrero, C.; Resendiz, J.; Ortega, A.

CORPORATE SOURCE: Inst. Quim., Univ. Nac. Auton. Mexico, Mexico City, Mex.

SOURCE: Revista Latinoamericana de Quimica (1978),  
9(3), 171-4  
CODEN: RLAQA8; ISSN: 0370-5943  
DOCUMENT TYPE: Journal  
LANGUAGE: Spanish  
GI

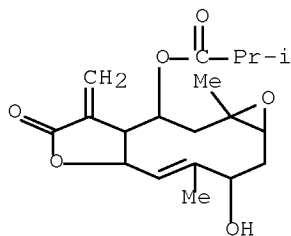


AB A new sesquiterpene lactone, viguiepinin (I), was isolated from *V. pinnatilobata* and its structure determined by IR, UV, and NMR spectroscopy of I and its acetylation, rearrangement, and reduction derivs. Ozic acid (II) was isolated from *V. stenoloba*. The structures of viguiestenin (III; R = Ac) and deacetylviguiestenin (III; R = H), constituents of *V. stenoloba*, were revised.

IT 59979-58-7P  
RL: PREP (Preparation)  
(from *Viguiera stenoloba*, structure revision of)

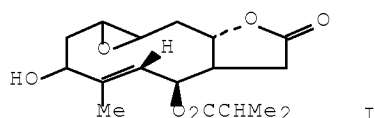
RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)

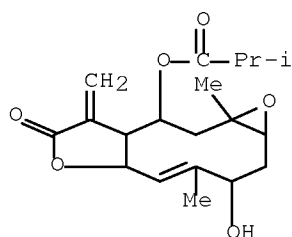


L75 ANSWER 57 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1978:62480 CAPLUS Full-text  
DOCUMENT NUMBER: 88:62480  
ORIGINAL REFERENCE NO.: 88:9875a,9878a  
TITLE: Chemical constituents of *Tithonia tagetiflora* Desf.:

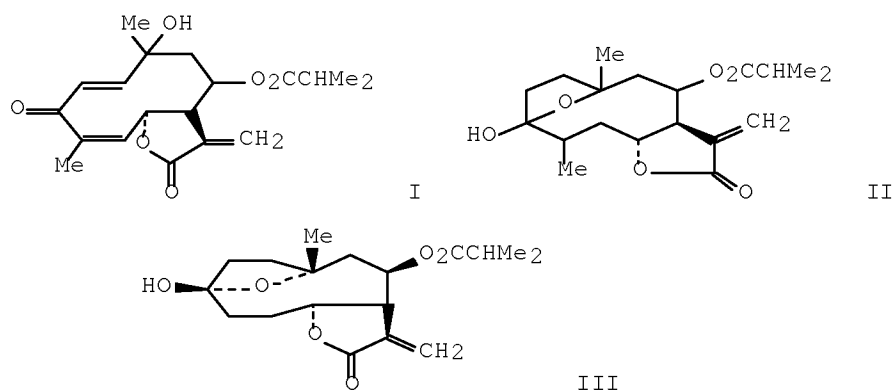
Part V. Structure of tagitinin E  
 AUTHOR(S): Pal, Raghwendra; Rastogi, R. P.  
 CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic  
 Chemistry Including Medicinal Chemistry (1977  
 ), 15B(6), 533-5  
 CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Tagitinin E, isolated from *T. tagetiflora* has structure I on the basis of  
 chemical reactions and <sup>1</sup>H NMR double resonance spectrometry. This is the only  
 tagitinin in which the lactone ring is fused at C-8.  
 IT 59979-58-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (of *Tithonia tagetiflora*, structure of)  
 RN 59979-58-7 CAPLUS  
 CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-  
 1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-  
 oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 58 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1977:498791 CAPLUS Full-text  
 DOCUMENT NUMBER: 87:98791  
 ORIGINAL REFERENCE NO.: 87:15669a,15672a  
 TITLE: Chemical constituents of *Tithonia tagetiflora* desf.:  
 part IV - tagitinin C, D and F  
 AUTHOR(S): Pal, Raghwendra; Kulshreshtha, D. K.; Rastogi, R. P.  
 CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic  
 Chemistry Including Medicinal Chemistry (1977  
 ), 15B(3), 208-11  
 CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The structure of tagitinins C, D and F, (I, II, and III, resp.) isolated from *T. tagitiflora*, were elucidated to be 12-carboxy-6,10-dihydroxy-8-isobutyryloxy-3-oxogermacra-1,4,11(13)-triene- $\gamma$ -lactone, 12-carboxy-3,6-dihydroxy-3,10-epoxy-8-isobutyryloxygermacra-11(13)-ene- $\gamma$ -lactone, and 12-carboxy-3,6-dihydroxy-3,10-epoxy-8-isobutyryloxygermacra-1,4,11(13)-triene- $\gamma$ -lactone, resp. on the basis of spectral data and chemical reactions. The structural and stereochem. relations among these substances as well as the correlation of I with tagitinin-B were established. I appears to be the 1st recognized naturally occurring germacranolide having trans-1,2-cis-4,5-diene system and III is among the few sesquiterpene lactones which show significant *in vivo* tumor inhibitory activity.

IT 59979-56-5 59979-57-6

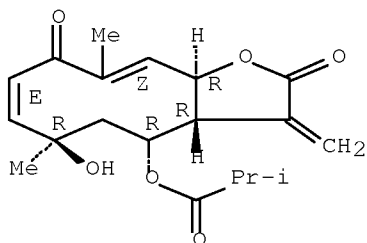
RL: BIOL (Biological study)  
(of *Tithonia tagitiflora*)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.

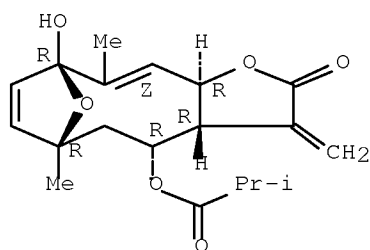


RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 59 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1976:472205 CAPLUS Full-text

DOCUMENT NUMBER: 85:72205

ORIGINAL REFERENCE NO.: 85:11539a,11542a

TITLE: Antileukemic and other constituents of *Tithonia tagitiflora* Desf.

AUTHOR(S): Pal, Raghwendra; Kulshreshtha, D. K.; Rastogi, R. P.

CORPORATE SOURCE: Div. Med. Chem., Cent. Drug Res. Inst., Lucknow, India

SOURCE: Journal of Pharmaceutical Sciences (1976), 65(6), 918-20

CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Phytochem. investigation of *T. tagitiflora* led to isolation of 6 new germacranolides, tagitinins A, B, C, D, E, and F,  $\beta$ -sitosterol [83-46-5], and  $\beta$ -D-glucoside [474-58-8]. Among these, tagitinin F [ 59979-57-6] possessed antileukemic activity.

IT 59979-56-5 59979-57-6 59979-58-7

RL: BIOL (Biological study)

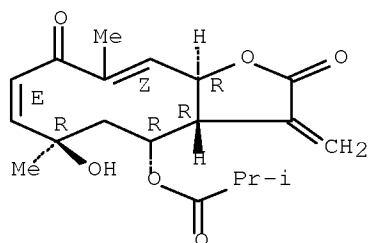
(isolation of, from *Tithonia tagitiflora*, neoplasm inhibition in relation to)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.

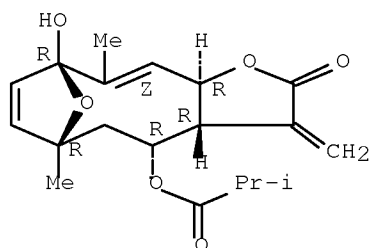


RN 59979-57-6 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,9R,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-6,9-epoxycyclodeca[b]furan-4-yl ester (CA INDEX NAME)

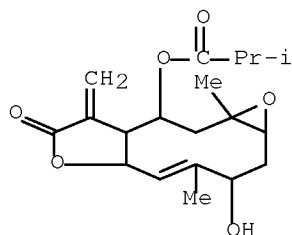
Absolute stereochemistry.

Double bond geometry as described by E or Z.



RN 59979-58-7 CAPLUS

CN Propanoic acid, 2-methyl-, (1aR,3S,4Z,5aR,8aR,9R,10aR)-  
1a,2,3,5a,7,8,8a,9,10,10a-decahydro-3-hydroxy-4,10a-dimethyl-8-methylene-7-  
oxooxireno[5,6]cyclodeca[1,2-b]furan-9-yl ester (9CI) (CA INDEX NAME)



L75 ANSWER 60 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1976:463182 CAPLUS Full-text

DOCUMENT NUMBER: 85:63182

ORIGINAL REFERENCE NO.: 85:10181a,10184a

TITLE: Chemical constituents of *Tithonia tagitiflora* Desf:  
Part II - Structure of tagitinin-B by application of  
homonuclear INDOR spectroscopy

AUTHOR(S): Pal, Raghwendra; Kulshreshtha, D. K.; Rastogi, R. P.

CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, India

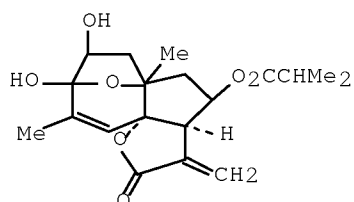
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1976  
, 14B(2), 77-80

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Tagitinin B, isolated from *T. tagitiflora*, has structure I on the basis of chemical reactions and internuclear double resonance and double NMR evidences. Its pos. Cotton effect has been attributed to the cis C(4)-C(5) double bond, which alters the dissymmetry effects.

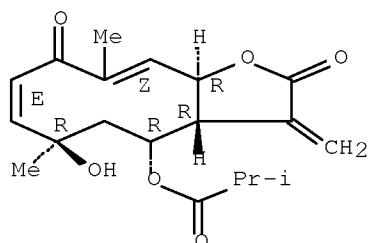
IT 59979-56-5F  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 59979-56-5 CAPLUS

CN Propanoic acid, 2-methyl-, (3aR,4R,6R,7E,10Z,11aR)-2,3,3a,4,5,6,9,11a-octahydro-6-hydroxy-6,10-dimethyl-3-methylene-2,9-dioxocyclodeca[b]furan-4-yl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L75 ANSWER 61 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:106318 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 70:106318

ORIGINAL REFERENCE NO.: 70:19839a,19842a

TITLE: Tumor inhibitors. XXXIII. Cytotoxic flavones from *Eupatorium* species

AUTHOR(S): Kupchan, S. Morris; Sigel, Carl W.; Hemingway, Richard J.; Knox, John R.; Udayamurthy, Muthu S.

SOURCE: Tetrahedron (1969), 25(8), 1603-15

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

AB From a cytotoxic extract of *E. semiserratum*, 5 flavones were isolated. Three of these were characterized as the previously known pectolinarigenin, and 2 new flavones, eupatorin and eupatilin. Structural studies are described which led to assignment of the 3',5-dihydroxy-4',6,7-trimethoxyflavone structure for eupatorin, and the 5,7-dihydroxy-3',4',6-trimethoxyflavone structure for eupatilin. From a cytotoxic extract of *E. cuneifolium*, 2 flavones were isolated, characterized as the previously known hispidulin and a new flavone, eupafolin. Structural studies are described which led to assignment of the 3',4',5,7-tetrahydroxy-6-methoxyflavone structure for eupafolin. The earlier assignment of this structure for pedalitin is shown to be incorrect, and the alternative 3',4',5,6-tetrahydroxy-7-methoxyflavone structure is proposed for pedalitin.

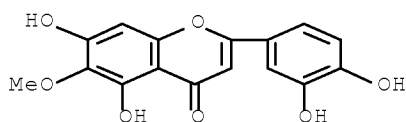
IT 520-11-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 520-11-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-methoxy-

(CA INDEX NAME)



L75 ANSWER 62 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1955:77871 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 49:77871

ORIGINAL REFERENCE NO.: 49:14752i,14753a

TITLE: New synthesis of luteolin 7-methyl ether

AUTHOR(S): Pankajamani, K. S.; Seshadri, T. R.

CORPORATE SOURCE: Univ. Delhi

SOURCE: J. Indian Chem. Soc. (1954), 31, 565

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

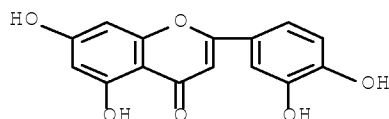
AB cf. C.A. 47, 4714e. Luteolin 7-Me ether (I) was prepared by the methylation of luteolin (II) in borate solution II was obtained from the SeO<sub>2</sub> oxidation of hesperidin (III). Thus, 6 g. III and 6 g. SeO<sub>2</sub> in 75 ml. Ac<sub>2</sub>O refluxed 4 hrs., filtered, and the filtrate poured into H<sub>2</sub>O gave diosmin acetate (IV), hydrolyzed with alc. HCl to diosmetin, which was dimethylated to 1.2 g. II. II (1 g.) in 150 ml. 5% borax treated over a period of 4 hrs. with 3 ml. Me<sub>2</sub>SO<sub>4</sub> and 40 ml. 5% NaOH, and the mixture filtered after 48 hrs., acidified, and extracted with ether gave 0.6 g. crude I, purified by preparation of the Pb salt, decomposition with H<sub>2</sub>S, and recrystn. from EtOH to give I as small yellow prisms, m. 260-2°. In circular paper chromatography with PhOH-H<sub>2</sub>O at 37° it gave a ring having R<sub>f</sub> value 1.

IT 491-70-3P, Luteolin

RL: PREP (Preparation)  
(preparation of)

RN 491-70-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



L75 ANSWER 63 OF 63 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1954:64305 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 48:64305

ORIGINAL REFERENCE NO.: 48:11404g-i,11405a-h

TITLE: Flavonoid glycosides of Dahlia variabilis. I. General introduction. Cyanidin, apigenin, and luteolin glucosides from the variety "Dandy"

AUTHOR(S): Nordstrom, C. G.; Swain, T.

CORPORATE SOURCE: Low Temp. Research Sta., Cambridge, UK

SOURCE: Journal of the Chemical Society (1953)  
2764-73

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE:

Journal

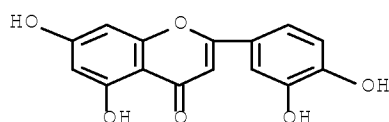
LANGUAGE:

Unavailable

AB A method for the identification of flavones and their glycosides on a micro scale is described. When applied to the compds. extracted from the flower of the blue dahlia "Dandy," the presence of 6 bands, containing apigenin (I), its 4'- (II) and 7-monoglucoside (III) and 7-rhamnoglucoside (IV), and the 5'-monoglucoside (V) and 7-diglucoside (VI) of luteolin; the arabinoglucoside of cyanidin (VII), and a few minor compds. has been demonstrated. Although the complex mixture of phenolic glucosides present in many petal exts. may readily be separated by paper chromatog., the individual compds. cannot usually be identified by their Rf values or color reactions alone. Attempts were therefore made to sep. the mixture before examination of the individual components. The authors have found that provided the solvent is removed from the developed paper chromatograms at room temperature individual bands can be quant. eluted in 24-48 h. with aqueous alc. These extracted bands may then be further purified, if necessary, by use of a 2nd solvent. Thus, (88.5 g.) of Dandy petals was crushed under 400 mL. 0.01N HCl-EtOH, kept at 0° 1 wk, ofiltered, the extract (10 mL.) applied as a streak from a teat pipet in 0.5-1 mL. portions to Whatman's Number 3 paper (22 + 18 in.), which had been previously washed 24 h. with H2O, in a chromatog. cabinet, dried at room temperature, the chromatogram developed overnight with BuOH-AcOH-H2O (6:1:2), carefully dried in a current of air in a fume cupboard, the position of the bands marked under an UV lamp, the separated components were eluted from the paper in a conventional chromatog. tank with either cold aqueous alc. (40-70%) for the flavones, or cold aqueous dilute HCl for the anthocyanins, and each of the resulting solns. was concentrated to a small volume in vacuo, purified by rerunning in the same solvent system, and eluted as before. The purified bands were then treated for homogeneity on Whatman's Number 1 paper in other solvents, and, when mixture, they were separated in a similar way so that used for the original extract Band 1 was eluted with 70% alc.; removal of most of the alc. left a dark brown solid, crystallizing from aqueous alc. in pale yellow crystals, m. 340°, identified as I, comparison of its Rf value, color reactions, and mixed m.p. with authentic synthetic I. Band 2 was shown to be a monoside by its RM value [ $RM = \log (1/Rf) - 1$ , varying directly with the number of functional groups], and on methylation (to determine the position of the sugar moiety) with Me2SO4, and anhydrous K2CO3 in dry Me2CO and subsequent hydrolysis yielded a compound, which, since it gave a neg. FeCl3 reaction, was presumably tetra-O-Me luteolin. Since gluosides in which the sugar is attached in the 4' or the 7-HO group in flavones are not affected under the above conditions, it appeared that band 2 was due to a 5'-glucoside. Upon methylation with CH2N2 it yielded a product giving a neg. FeCl3, test, and on hydrolysis with acid, the sugar-free Me ether gave a dark brown color with FeCl3, proving the presence of a 5'-HO group. Band 2 was V. Band 3 gave a mixture of components, separated in BuOH-H2O; and giving, when methylated and hydrolyzed, a product separated on impregnated paper with BuOH-H2O into 2 aglycons, whose Rf values and color reactions were identical with those of 4',5- and 5,7-di-O-methylapigenin. The spectra of this methylated product in 0.002M EtONa also indicated the presence of 2 components (II and III). III (cosmetin) had the same Rf value as authentic synthetic III in all solvents tried. II has not previously been reported. Band 4: the major component was shown to be a rhamnoglucoside of apigenin, and on quant. examination gave an apigenin: sugar ratio 1:2.2. Methylation followed by hydrolysis gave a product identical with 4',5-di-O-methylapigenin; partial hydrolysis gave IV, whose m.p., Rf value, color reaction, and spectra were identical with those of "rhoifolin." Band 5 yielded 2 components, the major component being a luteolin diglucoside. Methylation and hydrolysis showed that the sugar was at the 7-position and, unlike band 2, band 5 gave a brown color with FeCl3 solution before hydrolysis, showing the 5-HO group is free. Thus band 5 is VI. No compound of this nature has as yet been reported. The 2nd component gave on

hydrolysis glucose and a mixture of 2 aglycons, neither of which has as yet been identified. The anthocyanin band 6 was separated into 2 components with iso-PrOH-2N HCl. The major component on hydrolysis yielded cyanidin, arabinose, and glucose. It is probably a 3,5-diglucoside, but owing to fading of the aglycon at low concentration a quant. determination was not possible. The 2nd anthocyanin was present in too low a concentration for complete identification, but on hydrolysis gave an aglycon undistinguishable from pelargonidin. Tables of the Rf values and color reactions for the 6 bands are given.

IT 491-70-3P, Luteolin  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 491-70-3 CAPLUS  
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (CA INDEX NAME)



FILE 'HOME' ENTERED AT 15:37:14 ON 12 MAR 2008

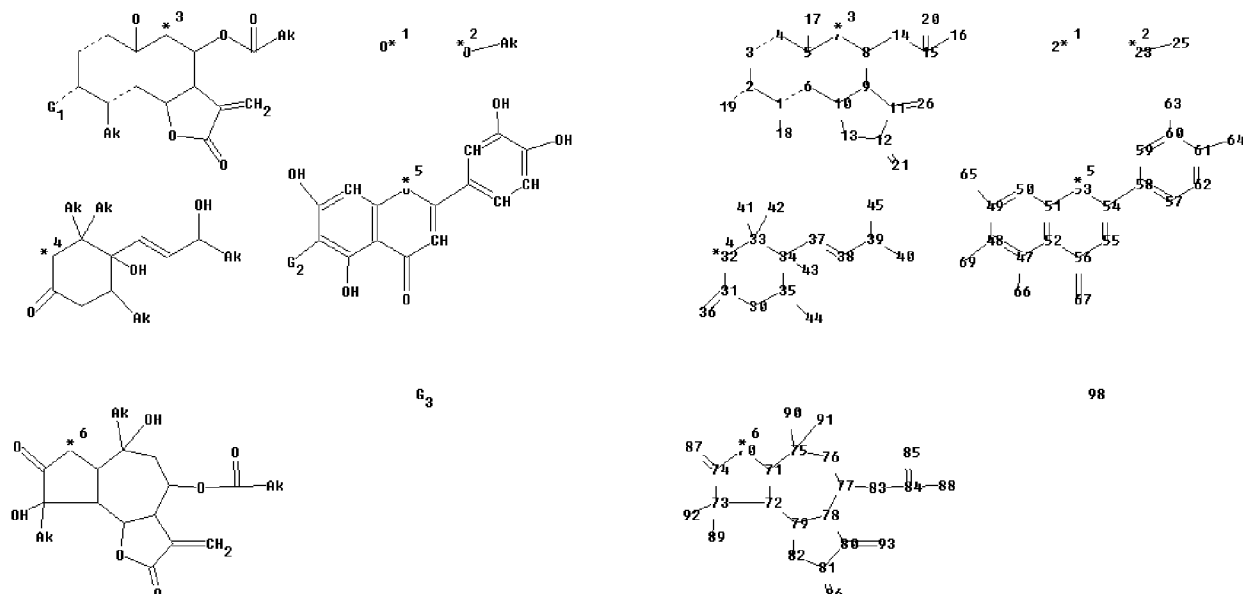
## SEARCH HISTORY

=> d stat que l49; d his nofile  
L5 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

Uploading L5.str



chain nodes :

14 15 16 18 19 20 21 22 23 25 26 36 37 38 39 40 41 42 43 44 45  
63 64 65 66 67 69 83 84 85 86 87 88 89 90 91 92 93 98

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 30 31 32 33 34 35 47 48 49 50  
51 52 53 54 55 56 57 58 59 60 61 62 70 71 72 73 74 75 76 77 78  
79 80 81 82

ring/chain nodes :

17

chain bonds :

1-18 2-19 8-14 11-26 12-21 14-15 15-16 15-20 23-25 31-36 33-41 33-42  
34-37 34-43 35-44 37-38 38-39 39-40 39-45 47-66 48-69 49-65 54-58 56-67  
60-63 61-64 73-89 73-92 74-87 75-90 75-91 77-83 80-93 81-86 83-84 84-85  
84-88

ring/chain bonds :

5-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-7 6-10 7-8 8-9 9-10 9-11 10-13 11-12 12-13 30-  
31 30-35 31-32 32-33 33-34 34-35 47-48 47-52 48-49 49-50 50-51 51-52  
51-53 52-56 53-54 54-55 55-56 57-58 57-62 58-59 59-60 60-61 61-62 70-71  
70-74 71-72 71-75 72-73 72-79 73-74 75-76 76-77 77-78 78-79 78-80 79-82  
80-81 81-82

exact/norm bonds :

1-2 1-6 1-18 2-3 2-19 3-4 4-5 5-7 6-10 7-8 8-9 8-14 9-10 9-11 10-13  
 11-12 12-13 12-21 14-15 15-16 15-20 23-25 31-36 33-41 33-42 34-43 35-44  
 39-40 39-45 47-66 48-69 49-65 51-53 52-56 53-54 54-55 55-56 56-67 60-63  
 61-64 70-71 70-74 71-72 71-75 72-73 72-79 73-74 73-89 73-92 74-87 75-76  
 75-90 75-91 76-77 77-78 77-83 78-79 78-80 79-82 80-81 81-82 81-86 83-84  
 84-85 84-88

exact bonds :

5-17 11-26 30-31 30-35 31-32 32-33 33-34 34-35 34-37 37-38 38-39 54-58  
 80-93

normalized bonds :

47-48 47-52 48-49 49-50 50-51 51-52 57-58 57-62 58-59 59-60 60-61 61-62

G1:[\*1],[\*2]

G2:H,MeO

G3:[\*3],[\*4],[\*5],[\*6]

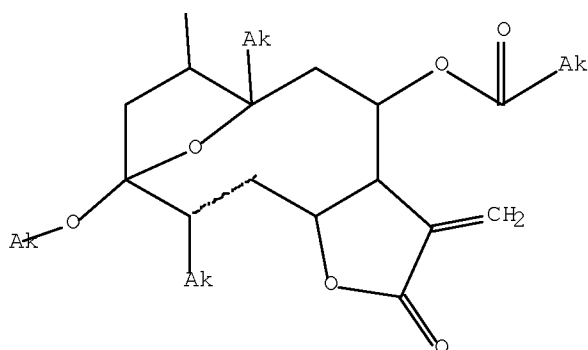
Connectivity :

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 25:1 E exact RC ring/chain 40:1 E exact RC ring/chain 41:1 E exact RC ring/chain  
 42:1 E exact RC ring/chain 44:1 E exact RC ring/chain 88:1 E exact RC ring/chain  
 89:1 E exact RC ring/chain 90:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:CLASS 30:Atom  
 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:CLASS 37:CLASS 38:CLASS 39:CLASS  
 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 47:Atom 48:Atom  
 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom  
 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 64:CLASS 65:CLASS 66:CLASS  
 67:CLASS 69:CLASS 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom  
 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:CLASS 84:CLASS 85:CLASS  
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 98:CLASS

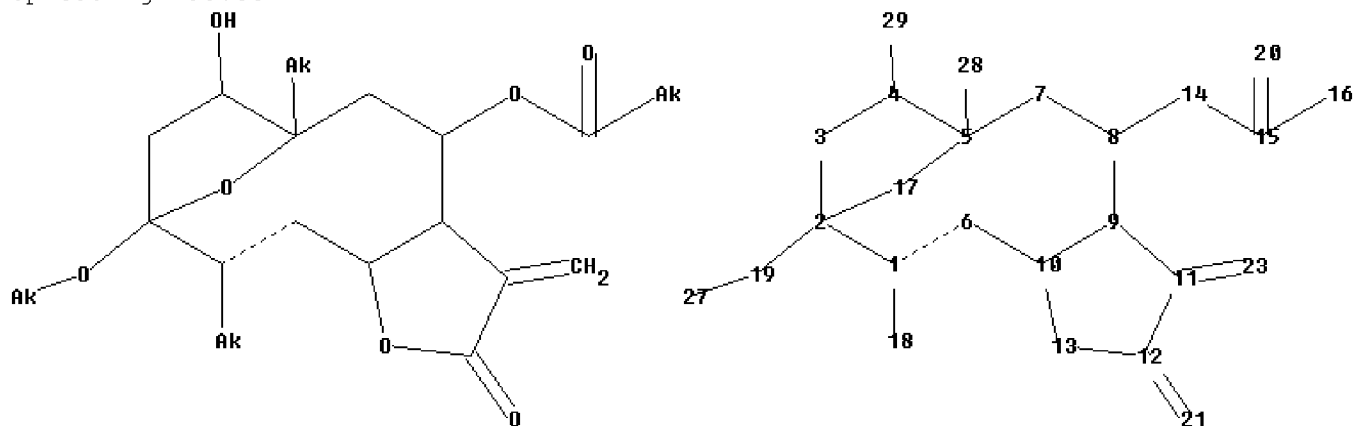
L8 237 SEA FILE=REGISTRY SSS FUL L5  
 L35 STR



G1  
 G2 H,MeO  
 G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L35.str



chain nodes :

14 15 16 18 19 20 21 23 27 28 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 17

chain bonds :

1-18 2-19 4-29 5-28 8-14 11-23 12-21 14-15 15-16 15-20 19-27

ring bonds :

1-2 1-6 2-3 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12 12-13

exact/norm bonds :

1-6 1-18 3-4 5-28 8-14 14-15 15-16 15-20 19-27

exact bonds :

1-2 2-3 2-19 2-17 4-5 4-29 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12 11-23 12-13 12-21

isolated ring systems :

containing 1 :

G1

G2:H,MeO

G3

Connectivity :

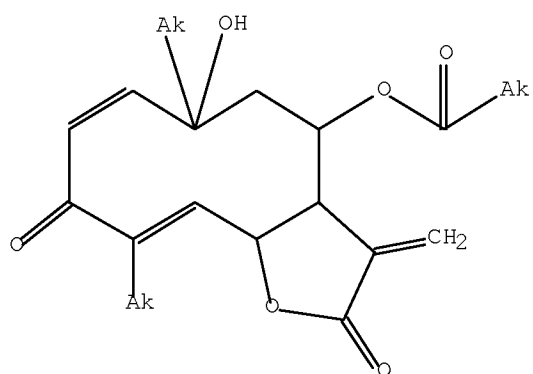
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18:1 E exact RC ring/chain 27:1 E exact RC ring/chain 28:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS 28:CLASS 29:CLASS

L36

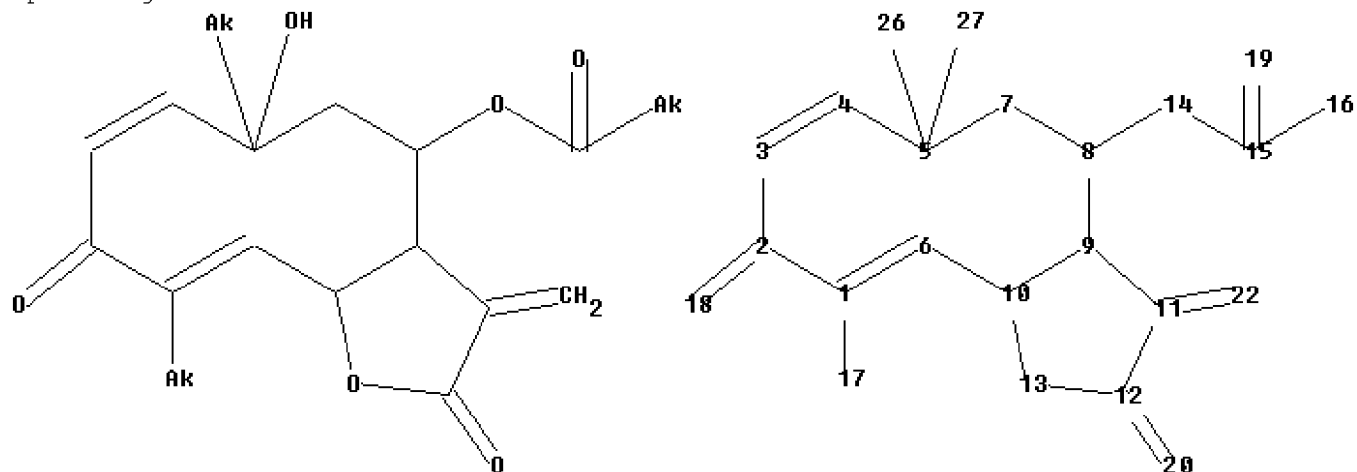
STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L36.str



chain nodes :  
14 15 16 17 18 19 20 22 26 27  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12 13  
chain bonds :  
1-17 2-18 5-26 5-27 8-14 11-22 12-20 14-15 15-16 15-19  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-7 6-10 7-8 8-9 9-10 9-11 10-13 11-12 12-13  
exact/norm bonds :  
1-17 2-18 5-26 8-14 12-20 14-15 15-16 15-19  
exact bonds :  
1-2 1-6 2-3 3-4 4-5 5-7 5-27 6-10 7-8 8-9 9-10 9-11 10-13 11-12 11-22  
12-13  
isolated ring systems :  
containing 1 :

G1

G2:H, MeO

G3

Connectivity :

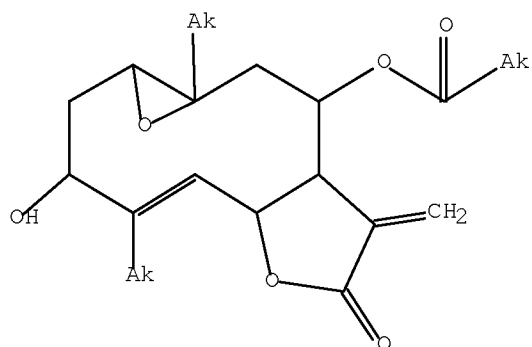
16:1 E exact RC ring/chain 17:1 E exact RC ring/chain 18:1 E exact RC ring/chain  
 26:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 22:CLASS 26:CLASS 27:CLASS

L37

STR



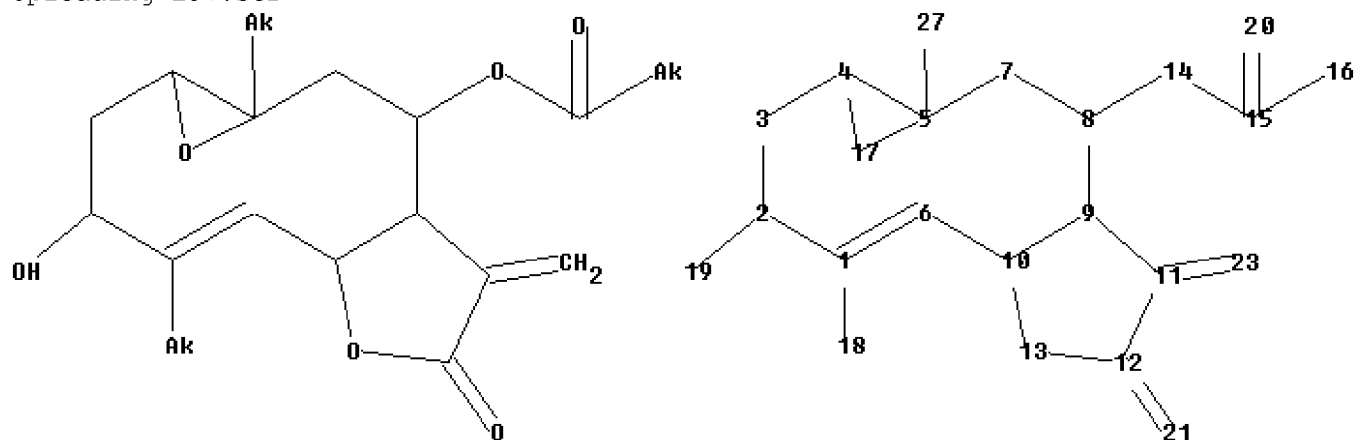
G1

G2 H, MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L37.str



chain nodes :

14 15 16 18 19 20 21 23 27

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 17

chain bonds :

1-18 2-19 5-27 8-14 11-23 12-21 14-15 15-16 15-20

ring bonds :  
 1-2 1-6 2-3 3-4 4-5 4-17 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12  
 12-13  
 exact/norm bonds :  
 1-18 5-27 8-14 14-15 15-16 15-20  
 exact bonds :  
 1-2 1-6 2-3 2-19 3-4 4-5 4-17 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13  
 11-12 11-23 12-13 12-21  
 isolated ring systems :  
 containing 1 :

G1

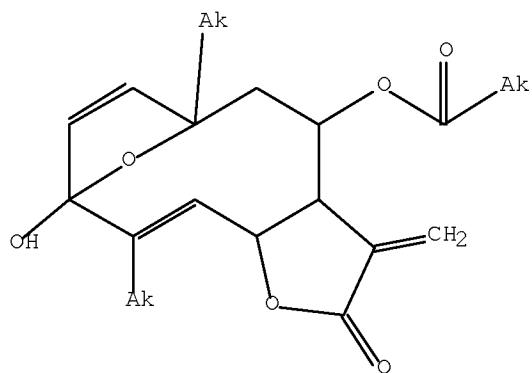
G2:H,MeO

G3

Connectivity :  
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 Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS

L38

STR



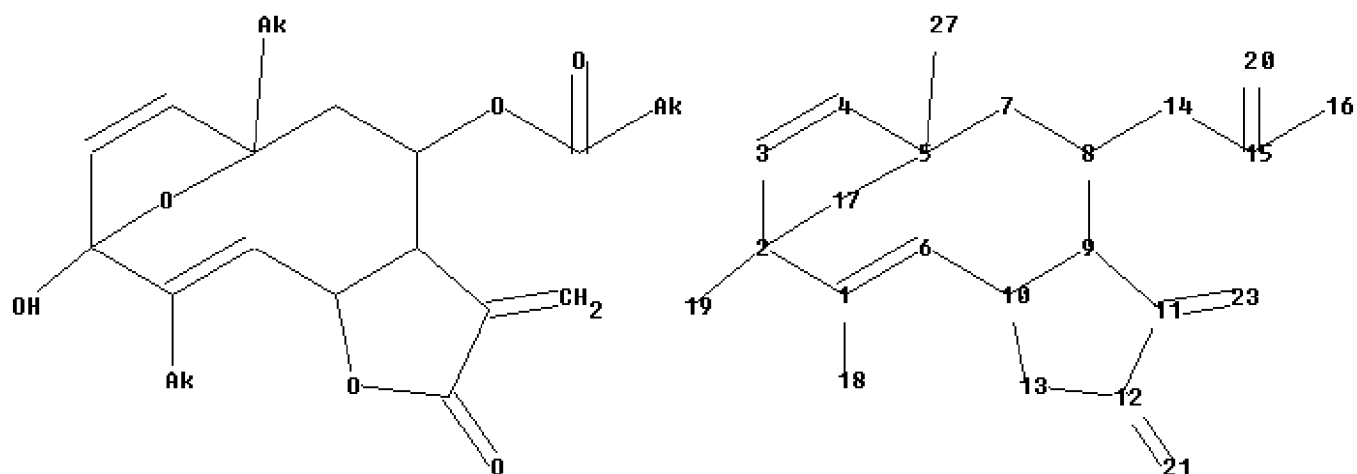
G1

G2 H,MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L38.str



```

chain nodes :
14 15 16 18 19 20 21 23 27
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 17
chain bonds :
1-18 2-19 5-27 8-14 11-23 12-21 14-15 15-16 15-20
ring bonds :
1-2 1-6 2-3 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13 11-12
12-13
exact/norm bonds :
1-18 5-27 8-14 14-15 15-16 15-20
exact bonds :
1-2 1-6 2-3 2-19 2-17 3-4 4-5 5-7 5-17 6-10 7-8 8-9 9-10 9-11 10-13
11-12 11-23 12-13 12-21
isolated ring systems :
containing 1 :

```

G1

G2:H, MeO

G3

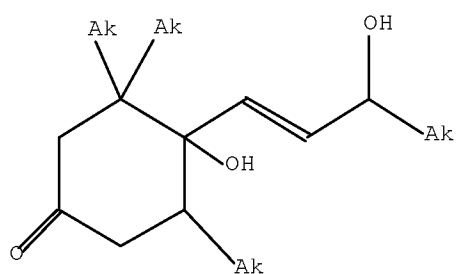
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Connectivity :
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19:CLASS 20:CLASS 21:CLASS 23:CLASS 27:CLASS

```

L39

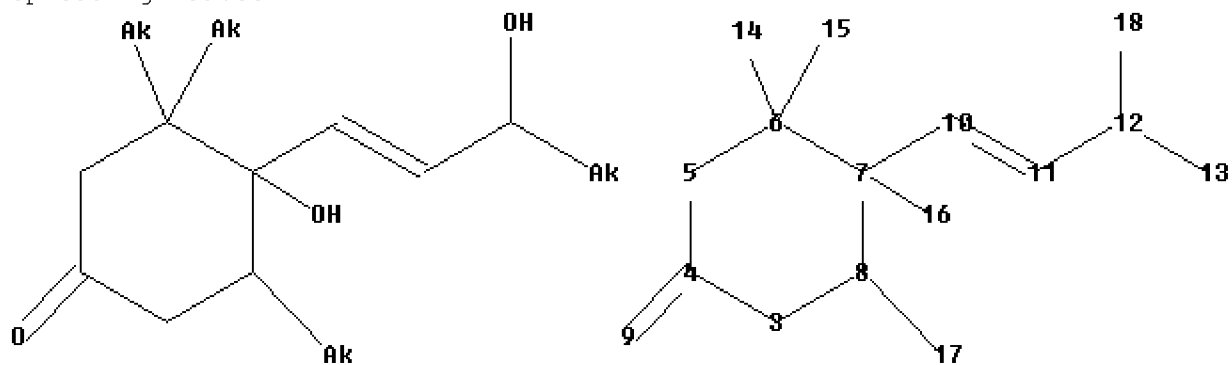
STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L39.str



chain nodes :  
9 10 11 12 13 14 15 16 17 18  
ring nodes :  
3 4 5 6 7 8  
chain bonds :  
4-9 6-14 6-15 7-10 7-16 8-17 10-11 11-12 12-13 12-18  
ring bonds :  
3-4 3-8 4-5 5-6 6-7 7-8  
exact/norm bonds :  
4-9 6-14 6-15 8-17 12-13  
exact bonds :  
3-4 3-8 4-5 5-6 6-7 7-8 7-10 7-16 10-11 11-12 12-18  
isolated ring systems :  
containing 3 :

G1

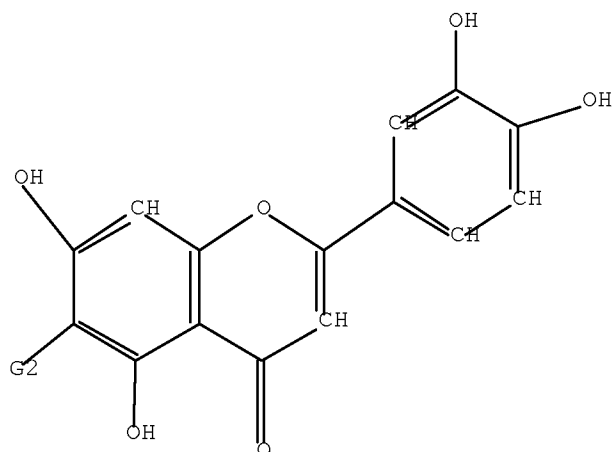
G2:H, MeO

G3

Connectivity :  
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:1 E exact RC ring/chain  
17:1 E exact RC ring/chain  
Match level :  
3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:CLASS

12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

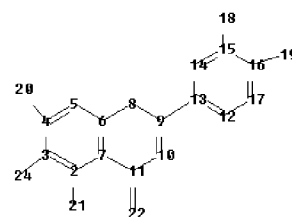
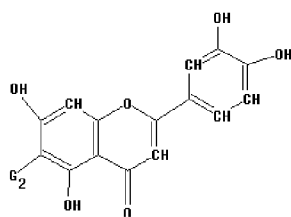
L40 STR



G1  
G2 H, MeO  
G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L40.str



chain nodes :

18 19 20 21 22 24

ring nodes :

2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-21 3-24 4-20 9-13 11-22 15-18 16-19

ring bonds :

2-3 2-7 3-4 4-5 5-6 6-7 6-8 7-11 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

2-21 3-24 4-20 11-22 15-18 16-19

exact bonds :

6-8 7-11 8-9 9-10 9-13 10-11

normalized bonds :

2-3 2-7 3-4 4-5 5-6 6-7 12-13 12-17 13-14 14-15 15-16 16-17

isolated ring systems :

containing 2 : 12 :

G1

G2:H, MeO

G3

Match level :

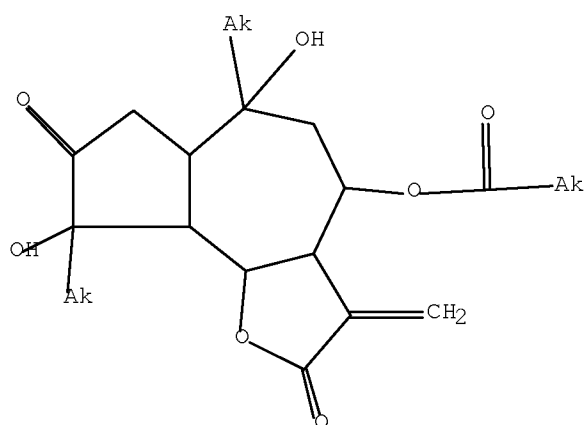
2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

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21:CLASS 22:CLASS 24:CLASS

L41

STR



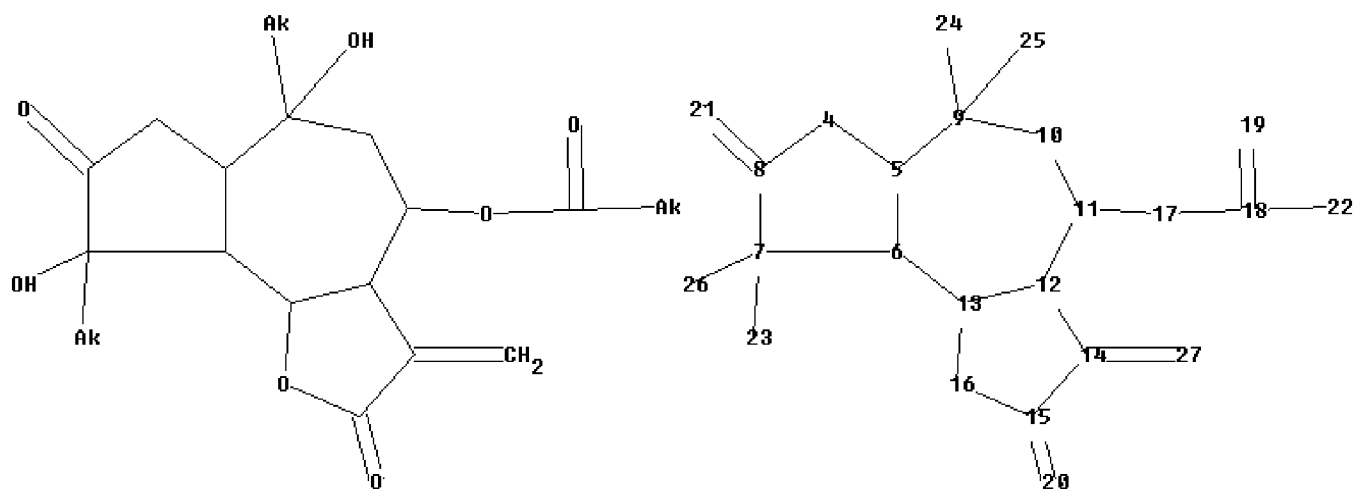
G1

G2 H, MeO

G3

Structure attributes must be viewed using STN Express query preparation.

Uploading L41.str



```

chain nodes :
17 18 19 20 21 22 23 24 25 26 27
ring nodes :
4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
7-23 7-26 8-21 9-24 9-25 11-17 14-27 15-20 17-18 18-19 18-22
ring bonds :
4-5 4-8 5-6 5-9 6-7 6-13 7-8 9-10 10-11 11-12 12-13 12-14 13-16 14-15
15-16
exact/norm bonds :
7-23 8-21 9-24 11-17 15-20 17-18 18-19 18-22
exact bonds :
4-5 4-8 5-6 5-9 6-7 6-13 7-8 7-26 9-10 9-25 10-11 11-12 12-13 12-14
13-16 14-15 14-27 15-16
isolated ring systems :
containing 4 :
```

G1

G2:H, MeO

G3

```

Connectivity :
22:1 E exact RC ring/chain 23:1E exact RC ring/chain 24:1 E exact RC ring/chain
Match level :
4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
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```

L44          65 SEA FILE=REGISTRY SUB=L8 SSS FUL (L35 OR L36 OR L37 OR L38 OR
              L39 OR L40 OR L41)
```

```

100.0% PROCESSED      181 ITERATIONS
SEARCH TIME: 00.00.01
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65 ANSWERS

(FILE 'HOME' ENTERED AT 11:13:14 ON 12 MAR 2008)

```

FILE 'REGISTRY' ENTERED AT 11:13:22 ON 12 MAR 2008
L1      STRUCTURE UPLOADED
L2      50 SEA SSS SAM L1

FILE 'STNGUIDE' ENTERED AT 11:14:12 ON 12 MAR 2008

FILE 'REGISTRY' ENTERED AT 11:17:11 ON 12 MAR 2008
L3      STRUCTURE UPLOADED
L4      50 SEA SSS SAM L3
        D STAT QUE L2

FILE 'STNGUIDE' ENTERED AT 11:18:21 ON 12 MAR 2008

FILE 'REGISTRY' ENTERED AT 11:20:38 ON 12 MAR 2008
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L6      13 SEA SSS SAM L5
L7      56321 SEA SSS FUL L5 EXTEND
L8      237 SEA SSS FUL L5
        SAVE TEMP L8 CHA588FULL/A

FILE 'CAPLUS' ENTERED AT 11:21:57 ON 12 MAR 2008
L9      4440 SEA ABB=ON  L8
        E US2006-580588/APPS
L10     2 SEA ABB=ON  US2006-580588/AP
L11     273 SEA ABB=ON  SASHIDA Y?/AU
L12     285 SEA ABB=ON  MIMAKI Y?/AU
L13     2087 SEA ABB=ON  KURODA M?/AU
L14     1638 SEA ABB=ON  KOBAYASHI R?/AU
L15     36 SEA ABB=ON  KANDO H?/AU
L16     198 SEA ABB=ON  NOSAKA K?/AU
L17     4933 SEA ABB=ON  ISHII H?/AU
L18     243 SEA ABB=ON  YAMORI T?/AU
L19     3 SEA ABB=ON  (L10 OR L11 OR L12 OR L13 OR L14 OR L15 OR L16 OR
        L17 OR L18) AND L9
        D SCAN
L20     ANALYZE L9 1- RN HIT :      232 TERMS
        D 1-20

FILE 'REGISTRY' ENTERED AT 11:25:47 ON 12 MAR 2008
L21     1 SEA ABB=ON  491-70-3
L22     236 SEA ABB=ON  L8 NOT L21

FILE 'CAPLUS' ENTERED AT 11:26:10 ON 12 MAR 2008
L23     590 SEA ABB=ON  L22

FILE 'REGISTRY' ENTERED AT 11:26:26 ON 12 MAR 2008
        D SCAN L21
L24     1 SEA ABB=ON  491-70-3

FILE 'CAPLUS' ENTERED AT 11:33:27 ON 12 MAR 2008
L25     4019 SEA ABB=ON  L21
L26     421 SEA ABB=ON  L23 NOT L25

FILE 'REGISTRY' ENTERED AT 11:33:59 ON 12 MAR 2008

FILE 'REGISTRY' ENTERED AT 11:34:50 ON 12 MAR 2008
L*** DEL      STRUCTURE UPLOADED
L27          STRUCTURE UPLOADED
L28          STRUCTURE UPLOADED

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L29 STRUCTURE UPLOADED  
 L30 STRUCTURE UPLOADED  
 L31 STRUCTURE UPLOADED  
 L32 STRUCTURE UPLOADED  
 L33 STRUCTURE UPLOADED  
 L34 5 SEA SUB=L8 SSS SAM (L27 OR L28 OR L29 OR L30 OR L31 OR L32 OR  
 L33)  
 D SCAN

FILE 'STNGUIDE' ENTERED AT 14:56:26 ON 12 MAR 2008

FILE 'REGISTRY' ENTERED AT 14:56:56 ON 12 MAR 2008

FILE 'STNGUIDE' ENTERED AT 14:57:28 ON 12 MAR 2008

FILE 'REGISTRY' ENTERED AT 15:06:58 ON 12 MAR 2008

L35 STRUCTURE UPLOADED  
 L36 STRUCTURE UPLOADED  
 L37 STRUCTURE UPLOADED  
 L38 STRUCTURE UPLOADED  
 L39 STRUCTURE UPLOADED  
 L40 STRUCTURE UPLOADED  
 L41 STRUCTURE UPLOADED  
 L42 4 SEA SUB=L8 SSS SAM (L35 OR L36 OR L37 OR L38 OR L39 OR L40 OR  
 L41)  
 L43 181 SEA SUB=L8 SSS FUL (L35 OR L36 OR L37 OR L38 OR L39 OR L40 OR  
 L41) EXTEND  
 L44 65 SEA SUB=L8 SSS FUL (L35 OR L36 OR L37 OR L38 OR L39 OR L40 OR  
 L41)  
 SAVE TEMP L44 CHA588SUB1/A

FILE 'CAPLUS' ENTERED AT 15:10:57 ON 12 MAR 2008

L45 4323 SEA ABB=ON L44

FILE 'REGISTRY' ENTERED AT 15:11:22 ON 12 MAR 2008

D SCAN L44  
 L46 STR  
 L47 1 SEA SUB=L44 SSS SAM L46  
 D SCAN  
 L48 15 SEA SUB=L44 SSS FUL L46 EXTEND  
 L49 10 SEA SUB=L44 SSS FUL L46  
 SAVE TEMP L49 CHA588SUB2/A  
 L50 30 SEA ABB=ON L44 AND BENZOPYRAN  
 D SCAN  
 SAVE TEMP L50 CHA588SUB3/A  
 E 3S  
 L51 328280 SEA ABB=ON 3S  
 L52 6 SEA ABB=ON L51 AND L44  
 D SCAN  
 L53 1 SEA ABB=ON L51 AND L44 AND 1/NR  
 SAVE TEMP L53 CHA588SUB4/A  
 L54 26 SEA ABB=ON L50 AND 1/NC  
 D SCAN

FILE 'CAPLUS' ENTERED AT 15:25:26 ON 12 MAR 2008

L55 50 SEA ABB=ON L49  
 L56 1 SEA ABB=ON L53  
 L57 4195 SEA ABB=ON L50  
 L58 3 SEA ABB=ON L57 AND (L11 OR L12 OR L13 OR L14 OR L15 OR L16 OR  
 L17 OR L18 OR L10)

D SCAN  
D PY L57 4195

FILE 'STNGUIDE' ENTERED AT 15:26:53 ON 12 MAR 2008

FILE 'REGISTRY' ENTERED AT 15:29:04 ON 12 MAR 2008

E 6/O

L59 12 SEA ABB=ON L50 AND (6-7/O)  
D SCAN  
L60 8 SEA ABB=ON L59 AND L54  
D SCAN  
L61 4 SEA ABB=ON L59 NOT L60  
D SCAN  
L62 2 SEA ABB=ON L59 AND (MONOHYDRATE OR SODIUM)  
L63 10 SEA ABB=ON (L60 OR L62)  
SAVE TEMP L63 CHA588SUB5/A

FILE 'CAPLUS' ENTERED AT 15:31:40 ON 12 MAR 2008

L64 4165 SEA ABB=ON L63  
D SCAN L58  
L65 449 SEA ABB=ON L63/P  
L66 395075 SEA ABB=ON CHROMATOG?/OBI  
L67 22 SEA ABB=ON L65 AND L66  
L68 50 SEA ABB=ON (L53 OR L49)  
L69 50 SEA ABB=ON L68 OR (L68 AND L64)  
L70 184654 SEA ABB=ON ANTITUMOR AGENTS/CT  
L71 482074 SEA ABB=ON NEOPLAS?/CW  
L72 28 SEA ABB=ON L65 AND (L70 OR L71)  
L73 98 SEA ABB=ON (L67 OR L69 OR L72)  
L74 64 SEA ABB=ON L73 AND (PY<2004 OR AY<2004 OR PRY<2004)

FILE 'CAPLUS' ENTERED AT 15:35:21 ON 12 MAR 2008

D QUE NOS L19  
D IBIB ABS HITSTR L19 1-3

FILE 'REGISTRY' ENTERED AT 15:36:28 ON 12 MAR 2008

D STAT QUE L44  
D STAT QUE L49  
D QUE NOS L53  
D QUE NOS L63

FILE 'CAPLUS' ENTERED AT 15:36:52 ON 12 MAR 2008

D QUE NOS L74  
L75 63 SEA ABB=ON L74 NOT L19  
D IBIB ABS HITSTR 1-63

FILE 'HOME' ENTERED AT 15:37:14 ON 12 MAR 2008

D STAT QUE L49

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